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ENERGY PRESERVING METHODS FOR VOLTERRA LATTICE EQUATION

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Abstract. We investigate linear energy preserving methods for the Volterra lattice equation as non-canonical Hamiltonian system. The averaged vector field method was applied to the Volterra lattice equation in bi-Hamiltonian form with quadratic and cubic Poisson brackets. Numerical results confirm the excellent long time preservation of the Hamiltonians and the polynomial integrals.

Keywords: Energy preserving integrators, Runge-Kutta methods, Bi-Hamiltonian systems, Poisson structure.

AMS Subject Classification: 65P10, 65L06, 37K10

1. Introduction

Traditionally, numerical integration of ordinary and partial differential equations concerns itself with the construction of numerical methods to minimize the global error, to ensure the numerical stability and to control the time step. In the last two decades, the concept of the design of numerical integrators shifted to preserve the intrinsic geometric properties, like to preserve the symplectic structure, symmetries, conserved quantities, the volume and phase space structure. These methods are known as geometric or structure preserving integrators. Most of the studies are concentrated in construction of symplectic and multisymplectic integrators for Hamiltonian ordinary and partial differential equations [12, 18, 24]. It is known that all Runge-Kutta methods preserve the linear integrals of the associated differential equations, and that only symplectic Runge-Kutta methods preserve the quadratic integrals. No Runge-Kutta method preserves higher order polynomial or nonlinear integrals. The symplectic structure and Hamiltonians can not preserved simultaneously, unless the integrator produces exact solutions (see [[12], page 379]).

Integrators that preserve the the energy or integrals have been considered since several decades. The development of the energy preserving methods started with the work of Courant, Friedrichs and Lewy [6]. They again gain attraction in recent years and several integral preserving methods for ordinary differential equations using discrete gradients and discrete variational derivatives [2, 3, 11, 21, 22, 23]. Discrete gradient methods were also applied to nonlinear evolutionary partial differential equations [7, 10]. There is also class of integrators which preserve exactly the energy of polynomial Hamiltonian systems

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[14, 15], which are known as "extended collocation methods" and "Hamiltonian Boundary Value Methods".

All methods mentioned above are non-linear, so that the numerical solution is not invariant with respect to the time transformation. Recently the so called average vector field method (AVF) attracted a lot of interest [19, 22] which is extension of the implicit mid-point rule. Higher order AVF methods are constructed by using the Guassian quadrature and they are interpreted as Runge-Kutta method with continuous stages. The AVF methods of arbitrarily higher order were developed and analyzed for canonical and non-canonical Hamiltonian systems in [13, 5]. A relation between the energy preservation and symplecticticness is established by so called B-series. A B-series for a system of ordinary differential equations is formal power series of the step size and elementary differential equations [2]. The discrete gradient methods for the integration of Hamiltonian systems can not be expanded in a B-series. Energy preserving B-series methods for canonical Hamiltonian systems were characterized in [1, 9]. The AVF method and its high order extension for canonical and non-canonical Hamiltonian systems [13, 5] are B-series methods. Using the B-series, it can shown that the AVF method for canonical and non-canonical Hamiltonian systems is conjugate to symplectic or Poisson integrators [13, 5]. Many partial differential equations like the Korteweg de Vries equation, non-linear Schrödinger equation, sine-Gordon equation can be recast as non-canonical Hamiltonian or Poisson systems. In the last two decades various symplectic and multi-symplectic integrators were successfully applied to Hamiltonian partial differential equations by preserving the integrals very accurately in long in term. Application of the AVF method for various nonlinear evolutionary partial differential equation was given in [4].

For non-canonical Hamiltonian systems, i.e for Poisson systems with the non-constant skew symmetric structure matrix, general structure preserving integrators are not available [17]. For example the implicit-mid point method which preserves the symplectic structure for canonical Hamiltonian systems is not a Poisson integrator. There exist only some geometric integrators which preserve the Poisson structure for some differential equations. For example the symplectic Euler method and partitioned Lobatto IIIA-IIIB methods preserve the Poisson structure of the Volterra lattice equation [8] and the integrable discretization of nonlinear Schrödinger equation [25]. In this paper we will apply the AVF method for non-canonical Hamiltonian systems in [5] to the Volterra lattice in bi-Hamiltonian form. Numerical results show the excellent energy preserving properties of the second and fourth order AVF method and fourth order energy preserving trapezoidal rule [14, 15] for the Volterra lattice equation with quadratic and cubic Poisson brackets.

The outline of the paper is as follows. In the next Section various energy preserving methods and their properties are given. In Section 3, we give the application of the AVF method to the Volterra lattice equation. Section 4 consists of numerical results with one and two stage AVF method and with the fourth order trapezoidal rule. The paper end with some conclusions and suggestions for a future work.

2. Energy preserving integrators

We consider the system of ordinary differential equations

$$y' = f(y), \quad y(0) = y_0 \in \mathbb{R}^n \tag{1}$$

with $f(y) = J(y)\nabla H$, where $J(y)$ is a $n \times n$ skew-symmetric structure matrix and H is an invariant, for example, the Hamiltonian or energy of the system. The energy preserving

discrete gradient methods rely on appropriate approximations of $\nabla H(y)$ and $J(y)$.

Symmetric discrete gradient methods for Poisson systems are given as [21, 22]

$$\frac{y^{n+1}-y^n}{h} = J\left(\frac{y^n+y^{n+1}}{2}\right)\cdot\overline{\nabla}H_s(y^n,y^{n+1}) \tag{2}$$

$$\overline{\nabla}H_s(y^n,y^{n+1}) := \frac{1}{2}\left(\overline{\nabla}H(y^n,y^{n+1})+\overline{\nabla}H(y^{n+1},y^n)\right)$$

with the coordinate increments

$$\overline{\nabla}H_s(y^n,y^{n+1}) := \begin{pmatrix} \frac{H(y_1^{n+1},y_2^n,\cdots y_i^n,\cdots,y_m^n)-H(y_1^n,y_2^n,\cdots y_i^n,\cdots,y_m^n)}{y_1^{n+1}-y_1^n} \\ \cdots \\ \frac{H(y_1^{n+1},y_2^{n+1},\cdots y_i^{n+1},\cdots,y_m^n)-H(y_1^{n+1},y_2^{n+1},\cdots y_i^n,\cdots,y_m^n)}{y_i^{n+1}-y_i^n} \\ \cdots \\ \frac{H(y_1^{n+1},y_2^{n+1},\cdots y_i^{n+1},\cdots,y_m^{n+1})-H(y_1^{n+1},y_2^{n+1},\cdots y_i^{n+1},\cdots,y_m^n)}{y_m^{n+1}-y_m^n} \end{pmatrix}.$$

Another class of energy preserving methods systems for polynomial Hamiltonians are $s-$stage the trapezoidal methods defined as [14, 15]

$$y^{n+1} = y^n + h\sum_{i=1}^{s} b_i J(K_i)\nabla H(K_i). \tag{3}$$

For $s=1$ it reduces to the implicit mid-point rule. The fourth order 3-stage method is given as [15]

$$\begin{aligned} y^{n+1} &= y^n \\ &+ \frac{h}{6}\left(J(y^n)\nabla H(y_n) + 4J\left(\frac{y^n+y^{n+1}}{2}\right)\nabla H\left(\frac{y^n+y^{n+1}}{2}\right) + J(y^{n+1})\nabla H(y^{n+1})\right). \end{aligned}$$

These methods are typically non-linear, so that the numerical solutions are not invariant with respect to the linear transformations, and in general can not be expanded as B-series, i.e. formal series for the system (1) in powers of the step size h and elementary differentials. The averaged vector field method for (1)

$$y^{n+1} = y^n + h\int_0^1 f(y^n+\tau(y^{n+1}-y^n))d\tau, \quad n=0,1,\cdots \tag{4}$$

is an extension of Runge-Kutta methods and admits B-series expansion. It is invariant with respect to linear transformations and it reduces to the discrete gradient method for canonical Hamiltonian systems.

Linear energy preserving average vector field integrators for Poisson systems are constructed [5]

$$y^{n+1} = y^n + hJ\left(\frac{y^n+y^{n+1}}{2}\right)\int_0^1 \nabla H(y^n+\tau(y^{n+1}-y^n))d\tau \tag{5}$$

as an extension of averaged vector field integrators for canonical Hamiltonian systems [13]

$$y^{n+1} = y^n + hJ\int_0^1 \nabla H(y^n+\tau(y^{n+1}-y^n))d\tau. \tag{6}$$

The AVF methods in [13, 5] are constructed by using the Gaussain quadrature similar to the symplectic Gauss-Legendre Runge-Kutta methods. They are interpreted as continuous-stage Runge-Kutta methods [13]

$$Y_\tau = y^n + h\int_0^1 a_{\tau,\sigma} f(Y_\sigma)\, d\sigma, \quad y^{n+1} = y^n + h\int_0^1 b_\sigma f(Y_\sigma)\, d\sigma, \tag{7}$$

for $\tau \in (0,1)$. Here, $Y_\tau \approx y(t_n + c_\tau h)$, where $c_\tau = \int_0^1 a_{\tau,\sigma}, d\sigma$. The integral stages Y_σ correspond to the values of the polynomial $y(t_n + \tau h)$ and the coefficients are given by

$$c_\tau = \tau, \quad a_{\tau,\sigma} = \sum_{i=1}^{s} \frac{1}{b_i}\int_0^\tau l_i(\alpha)\, d\alpha\, l_i(\sigma), \quad b_\sigma = 1. \tag{8}$$

with the basis polynomials of Lagrange interpolation at the collocation points $c_1, \cdots, c_s$

$$l_i(\tau) = \prod_{j=1, j\neq i}^{s} \frac{\tau - c_j}{c_i - c_j}, \qquad b_i = \int_0^1 l_i(\tau) d\tau.$$

Higher order linear integral preserving AVF methods, constructed using Gaussian quadrature for canonical and non-canonical Hamiltonian systems have even order $2s$ [13, 5].

For example, the AVF method (5-7) with $c_1 = 1/2$ as one stage Gaussian collocation method is an extension of the implicit mid-point rule. The two stage, fourth order Gaussian AVF integrator with

$$c_{1,2} = 1/2 \mp \sqrt{3}/6, \quad l_1(\tau) = (\tau - c_2)/(c_1 - c_2), \quad l_2(\tau) = (\tau - c_1)/(c_2 - c_1)$$

is given as [5]

$$\begin{aligned}
Y_1 &= y^n + h\int_0^1 \left(\frac{1}{2} l_1(\sigma) B(Y_1) + \left(\frac{1}{2} - \frac{\sqrt{3}}{3}\right) l_2(\sigma) B(Y_2)\right) \nabla H(Y_\sigma) d\sigma, \\
Y_2 &= y^n + h\int_0^1 \left(\left(\frac{1}{2} + \frac{\sqrt{3}}{3}\right) l_1(\sigma) B(Y_1) + \frac{1}{2} l_2(\sigma) B(Y_2)\right) \nabla H(Y_\sigma) d\sigma, \\
y^{n+1} &= y^n + h\int_0^1 \left(l_1(\sigma) B(Y_1) + l_2(\sigma) B(Y_2)\right) \nabla H(Y_\sigma) d\sigma.
\end{aligned} \tag{9}$$

Gaussian AVF methods are time-symmetric and conjugate to symplectic integrators. A numerical one-step method $y^{n+1} = \Phi_h(y^n)$ time-symmetric such that $y^n = \Phi_{-h}(y^{n+1})$ when applied to reversible systems (e.g. Hamiltonian systems). AVF methods are time-symmetric [13]. B-series integrators like the AVF method, which preserve exactly conserve the energy for Hamiltonian systems are not symplectic. But the AVF methods of order $2s$ are are conjugate-symplectic up to order $2s+2$, i.e. there exist a change of coordinates $\Psi(y) = y + \mathcal{O}(h^{2s})$, such that $\Psi_h^{-1} \circ \phi_h \circ \Psi_h$ is symplectic integrator [13].

3. Volterra lattice equations

The m-dimensional Volterra lattice

$$\dot{y}_i = y_i(y_{i+1} - y_{i-1}), \quad i = 1, \ldots, m \tag{10}$$

with periodic boundary conditions $y_{m+i} = y_i$, represents an integrable discretization of the Korteweg de Vries (KdV) equation and of inviscid Burger's equation and describes many phenomena such as the vibrations of particles on lattices, waves in plasmas and the

evolution of populations in a hierarchical system of competing species [8]. The Volterra lattice equations (10) have a bi-Hamiltonian structure [8]

$$\dot{y} = J_0(y)\nabla H_1 = J_1(y)\nabla H_0 \tag{11}$$

with respect to the quadratic and the cubic Poisson brackets

$$\{y_i, y_{i+1}\}_0 = y_i y_{i+1}, \quad \{y_i, y_{i+1}\}_1 = y_i y_{i+1}(y_i + y_{i+1}), \quad \{y_i, y_{i+2}\}_1 = y_i y_{i+1} y_{i+2}. \tag{12}$$

The corresponding Hamiltonians are

$$H_1 = \sum_{i=1}^{m} y_i, \qquad H_0 = \frac{1}{2}\sum_{i=1}^{m} \log(y_i). \tag{13}$$

The structure matrix $J_0(x)$ corresponding to the quadratic is a cyclic tridiagonal matrix.

$$J_0(y) = \begin{pmatrix} 0 & y_1y_2 & \dots & \dots & -y_1y_m \\ \vdots & \ddots & \ddots & \ddots & 0 \\ \dots & -y_{i-1}y_i & 0 & y_iy_{i+1} & \dots \\ \vdots & \vdots & \dots & \vdots & \vdots \\ y_1y_m & \dots & \dots & -y_{m-1}y_m & 0 \end{pmatrix}.$$

Similarly the structure matrix $J_1(x)$ corresponding to the cubic Possion bracket is a cyclic pentadiagonal matrix.

If the Poisson brackets are compatible, i.e. the sum of $\{\cdot,\cdot\}_0 + \{\cdot,\cdot\}_1$ is again a Poisson bracket, then the bi-Hamiltonian system (1) has a finite number of functionally independent first integrals $I_i, i = 1, \dots, m$ in involution i.e. $\{I_i, I_j\}_k = 0$ for $k = 0, 1$ and $i \neq j$, i.e.. the Volterra lattice is completely integrable with respect to both brackets.

Additional conserved quantities of the Volterra lattice (10) are the quadratic and cubic integrals [8].

$$I_q = \sum_{i=1}^{m} \frac{1}{2}y_i^2 + y_i y_{i+1}, \quad I_c = \sum_{i=1}^{m} \frac{1}{3}y_i^3 + y_i y_{i+1}(y_i + y_{i+1} + y_{i+2}). \tag{14}$$

In discretized form, the Hamiltonian H_1, I_q, I_c correspond to the mass, momentum and energy integrals of the KdV equation.

A function function $P(y)$ is called a distinguished or Casimir function, if $\{P, F\} =$ for any function $F(y)$. The Hamiltonian H_0 is a Casimir with respect to the Poisson bracket $\{\cdot,\cdot\}_0$, i.e.$\{H_0, F\}_0 = 0$. It was shown in [5] that the AVF integrators based on the Gaussian quadrature exactly preserves the quadratic Casimirs $P(y) = y^T Ay$ with a constant symmetric matrix A.

When the symmetrized discrete gradient method (2), the AVF method (6) and one stage trapezoidal method is applied to the Volterra lattice (11) with with quadratic brackets, i.e with $J_0(y)$ and $H_1(y)$, the implicit mid-point method is obtained.

Nonlinear implicit equations resulting by from application of the AVF method (6) to the Volterra lattice (11)

$$y^{n+1} - y^n - hF(y^{n+1}, y^n) = 0$$

are solved usually by Newton's method

$$(I - \frac{h}{2}F'(y_k^n))(y_{k+1}^{n+1} - y_k^{n+1}) = -hF(y_k^n), \quad k = 0, 1, \cdots$$

where k denotes the iteration index, and $F'(y_k^n)$ the Jacobian evaluated at y_k^n As starting value in the Newton iteration $y_0^{n+1} = y^n$ is taken.

Application of two stage linear energy preserving AVF method (10) to the Volterra lattice (11) gives

$$\begin{aligned} Y_1 &= y_0 + h(a_{11}B(Y_1) + a_{12}B(Y_2)) \\ Y_2 &= y_0 + h(a_{21}B(Y_1) + a_{22}B(Y_2)) \end{aligned}$$

$$\begin{aligned} a_{11} &= \tfrac{1}{2}\left(\tfrac{1}{2}\tfrac{1}{c_1-c_2} - \tfrac{c_2}{c_1-c_2}\right), & a_{12} &= \left(\tfrac{1}{2} - \tfrac{\sqrt{3}}{2}\right)\left(\tfrac{1}{2}\tfrac{1}{c_2-c_1} - \tfrac{c_1}{c_2-c_1}\right), \\ a_{21} &= \left(\tfrac{1}{2} + \tfrac{\sqrt{3}}{2}\right)\left(\tfrac{1}{2}\tfrac{1}{c_1-c_2} - \tfrac{c_2}{c_1-c_2}\right), & a_{22} &= \tfrac{1}{2}\left(\tfrac{1}{2}\tfrac{1}{c_2-c_1} - \tfrac{c_1}{c_2-c_1}\right). \end{aligned}$$

Application of the Newton method results in

$$\begin{aligned} &\begin{pmatrix} I - ha_{11}F'(Y_{1,k}) & -ha_{12}F'(Y_{2,k}) \\ -ha_{21}F'(Y_{1,k}) & I - ha_{22}F'(Y_{2,k}) \end{pmatrix} \begin{pmatrix} Y_{1,k+1} - Y_{1,k} \\ Y_{2,k+1} - Y_{2,k} \end{pmatrix} \\ = \; & -h \begin{pmatrix} a_{11}B(Y_{1,k}) + a_{12}B(Y_{2,k}) \\ a_{21}B(Y_{1,k}) + a_{22}B(Y_{2,k}) \end{pmatrix} \quad , k = 0, 1, \cdots \end{aligned}$$

with the starting values $Y_{1,0} = Y_{2,0} = y^n$. Compared with the one stage method, a linear system with a two by two block matrix have to solved at each iteration step, which shows that higher order Gaussian AVF methods are computationally expensive.

4. Numerical Results

For the periodic Volterra lattice we have used the following initial condition

$$y(x_i) = 1 + (1/2m^2)\,\mathrm{sech}^2(x_i), \quad x_i = -1 + (i-1)(1/2m^2), \quad i = 1, \ldots, m$$

All computations are done with a constant time step $h = 0.1$ for a Volterra lattice of dimension $m = 40$. In the case of quadratic brackets, the unknowns are in quadratic form. Therefore one Newton iteration was sufficient to solve for the unknowns. In the case of the cubic Poisson bracket, several Newton iterations are needed to solve the implicit equations accurately. Also the integral terms will be undefined when y^n is used as a starting value in the Newton iteration, therefore the limit of the integral is used for the first Newton step.

Long term preservation of the linear and logarithmic Hamiltonians (14), quadratic and cubic integrals (15) computed with the one stage linear energy preserving integrator (6) are shown in In Figure 1 & 2. In Table 1, the errors in the mean square root norm are given $\sqrt{\sum_{i=1}^{N}(I^i - I_0)^2/N}$, where I^i denote the computed Hamiltonians or first integrals at time step t_i and N is the number of time steps. Table 1 shows that the Hamiltonians and integrals are preserved within the machine accuracy for the quadratic brackets. The conserved quantities for the cubic Poisson bracket are preserved less accurately than for the quadratic brackets. But there is no drift in long term integration using both brackets in Figure 1 & 2.

In Table 2, in Figure & 4, numerical results with two stage AVF method (10) and fourth order trapezoidal method (4) are given for the quadratic bracket. These results shows the

excellent energy preservation of higher order AVF methods.

The logarithmic Hamiltonian H_0 as a Casimir for the Volterra lattice with quadratic bracket is also well preserved in Figure 1 and 3 in long term integration. Therefore the one and two stage AVF integrators (6) and (10) are conjugate to a Poisson integrator.

A comparison of results obtained with the symplectic Euler and Lobatto IIIA-B in [8] shows, that the AVF method preserve the Casimir H_0 and the quadratic and cubic integrals I_q, I_c more accurately.

TABLE 1. Average errors of the Hamiltonians and first integrals

	quadratic Poisson structure				cubic Poisson structure			
Δt	H_1	H_0	I_q	I_c	H_1	H_0	I_q	I_c
1/5	1.7e-16	8.7e-17	5.3e-16	2.4e-15	2.6e-8	1.3e-8	7.5e-8	2.6e-7
1/10	2.2e-16	1.1e-16	6.7e-16	2.2e-15	1.9e-9	9.5e-10	5.7e-9	1.9e-8
1/20	1.5e-16	6.9e-17	4.4e-16	1.4e-15	1.3e-8	6.7e-9	3.9e-8	1.3e-7

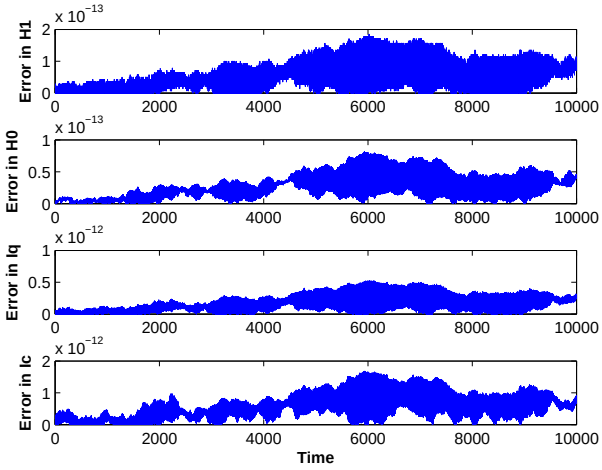

FIGURE 1. One stage AVF with quadratic Poisson brackets

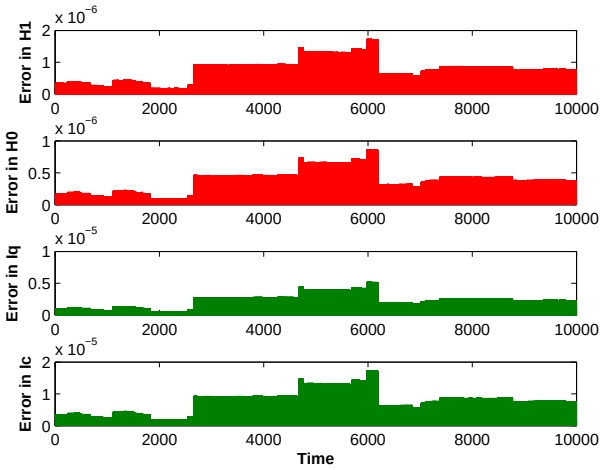

FIGURE 2. One stage AVF method with cubic Poisson brackets

	two stage trapezoidal rule				Two stage AVF method			
Δt	H_1	H_0	I_q	I_c	H_1	H_0	I_q	I_c
1/5	1.3e-16	7.1e-17	8.5e-16	6.7e-15	2.1e-20	2.1e-16	6.0e-16	3.1e-15
1/10	1.6e-16	6.4e-17	4.6e-16	1.6e-15	2.0e-20	4.0e-16	1.2e-15	4.4e-15
1/20	9.4e-17	4.4e-17	2.6e-16	8.8e-16	2.3e-21	9.3e-17	2.6e-16	9.3e-16

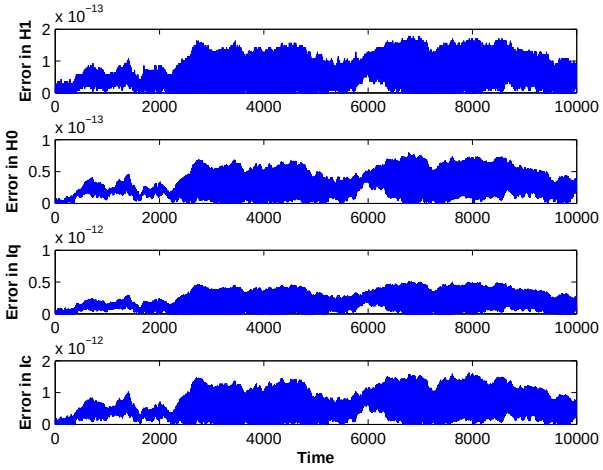

FIGURE 3. Two stage trapezoidal method

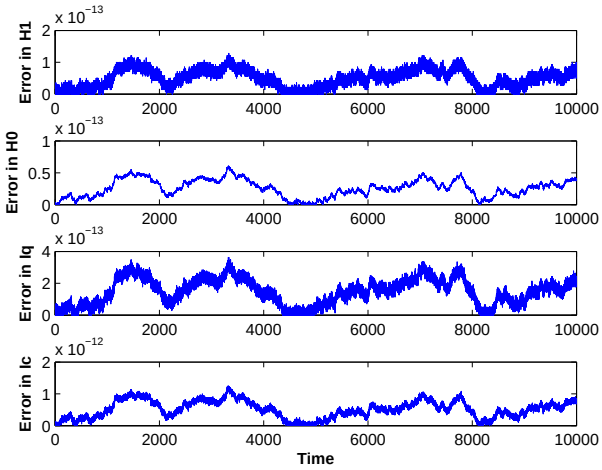

FIGURE 4. Two stage AVF method

5. Conclusions

All computations show that the Hamiltonians, quadratic and cubic integrals are preserved with a high accuracy, for the quadratic Poisson bracket better than for the cubic Poisson bracket. It is known that the Hamiltonians and the Poisson structure can not be preserved by any integrator at the same time. But, we can conclude that the AVF for the Volterra lattice equation are conjugate to a Poisson integrator, because there is no drift in long term preservation of the Hamiltonians.

One of the problem of the AVF method is the computation of the integrals. For polynomial vector fields the integrals can be computed exactly at the begin of integration and the complexity of the AVF method is comparable with the implicit Runge–Kutta methods. For the Volterra lattice, for the second Hamiltonian formulation, the logarithmic terms were integrated exactly too. Because the energy preserving methods are implicit as symplectic and multisymplectic integrators, the resulting nonlinear equations must be solved to within round-off error, to preserve symplecticity or the energy. This limits the applicability of these methods to large scale systems. In [20] a Newton-Taylor iteration was proposed to solve the implicit equations of symplectic Runge-Kutta methods, using the Jacobian of the vector field. This method preserve the symplectic structure at large time steps using only matrix-vector multiplications in each iteration. Similarly for energy preserving method, linearly implicit are used which require the solution of precisely one linear system of equations in each time step [7] and makes the energy preserving methods more efficient.

Another interesting lattice equation is the Ablowitz-Ladik integrable discretization of non-linear Schrödinger (IDNLS) equation [25] which has quadratic Poisson bracket as the Volterra lattice and the Hamiltonian contains quadratic and logarithmic terms. We plan to apply the AVF method to IDNLS equation.

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