BIT manuscript No.
(will be inserted by the editor)

Linear energy-preserving integrators for Poisson systems

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Received: date / Accepted: date

Abstract For Hamiltonian systems with non-canonical structure matrix a new class of numerical integrators is proposed. The methods exactly preserve energy, are invariant with respect to linear transformations, and have arbitrarily high order. Those of optimal order also preserve quadratic Casimir functions. The discussion of the order is based on an interpretation as partitioned Runge–Kutta method with infinitely many stages.

Keywords Poisson system · energy preservation · Casimir function · partitioned Runge–Kutta method · collocation · Gaussian quadrature

PACS 45.20.Jj · 02.30.Hq · 02.60.Lj

Mathematics Subject Classification (2000) 65P10 · 65L06

1 Introduction

We consider non-canonical Hamiltonian systems

$$\dot{y} = B(y)\nabla H(y), \qquad y(t_0) = y_0, \tag{1.1}$$

where $B(y)$ is a skew-symmetric matrix, so that the energy $H(y)$ is preserved along exact solutions of (1.1). In this article we do not require that $B(y)$ satisfies the Jacobi identity. Our main interest is the design of numerical integrators that exactly preserve the Hamiltonian $H(y)$ and are invariant with respect to linear transformations.

This work was partially supported by the Fonds National Suisse, project No. 200020-126638.

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There is a lot of research activity in energy preserving numerical integrators, and various discrete gradient methods have been proposed in the literature, see [2,8]. For these methods the numerical solution is typically not invariant with respect to arbitrary linear transformations. More recently, linear energy preserving integrators have been proposed for canonical Hamiltonian systems. The averaged vector field method [8,9] extends the implicit mid-point rule and requires the accurate computation of integrals. The article [7] presents Runge–Kutta methods that preserve the energy for polynomial Hamiltonians. An extension of the averaged vector field integrator to arbitrarily high order is proposed and analyzed in [4]. Until now, energy preserving integrators for non-canonical Hamiltonian systems that are invariant with respect to linear transformations, do not seem to exist.

The present article is devoted to an extension of the methods introduced in [4] to problems of the form (1.1). The most simple example is

$$y_1 = y_0 + hB\Big(\frac{y_0+y_1}{2}\Big)\int_0^1 \nabla H\big(y_0+\tau(y_1-y_0)\big)\,\mathrm{d}\tau \tag{1.2}$$

which reduces to the averaged vector field integrator for the case where $B(y)$ is a constant matrix. Note that this method treats the factors $B(y)$ and $\nabla H(y)$ in (1.1) differently, and should thus be considered as a partitioned method. As will be shown, this scheme exactly preserves energy and quadratic Casimir functions, it is symmetric and of order 2.

The new class of methods is presented in Section 2. It is a variant of classical collocation methods. Section 3 studies and proves properties such as exact preservation of energy and Casimir functions, symmetry, and invariance with respect to linear transformations. An interpretation of the proposed methods as partitioned Runge–Kutta methods is given in Section 4. This allows one to get information on the correct order of convergence. Numerical experiments are presented in Section 5.

2 Energy-preserving integration methods

We present a class of numerical time integrators that exactly preserve the energy $H(y)$, are invariant with respect to linear coordinate transformations, and are of arbitrarily high order.

2.1 Definition of the numerical integrator

Motivated by classical collocation methods, we start by considering an s-point quadrature formula with nodes c_i. The corresponding weights b_i can be obtained from the Lagrange basis polynomials in interpolation as follows:

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

Definition 2.1 (Energy-preserving integrator) Let $c_1,\dots,c_s$ be distinct real numbers (usually $0 \le c_i \le 1$) for which $b_i \neq 0$ for all i. We consider a polynomial $u(t)$ of degree s satisfying

$$u(t_0) = y_0 \tag{2.1}$$

$$\dot{u}(t_0 + c_j h) = B\big(u(t_0 + c_j h)\big) \int_0^1 \frac{\ell_j(\tau)}{b_j} \nabla H\big(u(t_0 + \tau h)\big)\, \mathrm{d}\tau. \tag{2.2}$$

The numerical solution after one step is then defined by $y_1 = u(t_0 + h)$.

Note that approximating the integral by the quadrature formula with nodes c_i and weights b_i reduces the integrator to a classical collocation method. For quadratic Hamiltonians the integrand in (2.2) is polynomial of degree $2s-1$, so that for Gauss points c_i (zeros of shifted Legendre polynomial) classical collocation is obtained for general $B(y)$. This integrator treats the arguments in $B(y)$ and in $\nabla H(y)$ differently and can thus be considered as a partitioned numerical method. The numerical solution therefore depends on the particular factorization of the vector field.

If $B(y) = B$ is a constant matrix (e.g., if (1.1) is a canonical Hamiltonian system), the method becomes the energy-preserving integrator of [4].

2.2 Implementation issues

If we denote $Y_\tau := u(t_0 + \tau h)$ and, with abuse of notation, $Y_j := u(t_0 + c_j h)$, Lagrange interpolation shows that

$$\dot{u}(t_0 + \tau h) = \sum_{j=1}^{s} \ell_j(\tau) B(Y_j) \int_0^1 \frac{\ell_j(\sigma)}{b_j} \nabla H\big(Y_\sigma\big)\, \mathrm{d}\sigma, \tag{2.3}$$

and by integration we arrive at

$$Y_\tau = y_0 + h \sum_{j=1}^{s} \int_0^1 \Big(\frac{\ell_j(\sigma)}{b_j} \int_0^\tau \ell_j(\alpha)\, \mathrm{d}\alpha \Big) B(Y_j) \nabla H\big(Y_\sigma\big)\, \mathrm{d}\sigma. \tag{2.4}$$

The polynomial $u(t)$ of degree s can be expressed in terms of y_0 and $Y_1,\dots,Y_s$. Therefore, we need equation (2.4) only for $\tau = c_i$ $(i = 1,\dots,s)$ to compute this polynomial. This represents a nonlinear system of equations for the unknowns $Y_1,\dots,Y_s$ which can be solved by iteration. The complexity is similar to that for implicit Runge–Kutta methods with s stages, and identical to that of the energy-preserving integrators of [4].

2.3 Examples

Methods of optimal order will be obtained when $c_1,\dots,c_s$ are the zeros of the sth Legendre polynomials. The corresponding quadrature formula (Gauss formulas) are of order $r = 2s$.

Case $s = 1$. We have $c_1 = 1/2$ and obtain the method (1.2). It is symmetric, of order two, and is an extension of the implicit mid-point rule.

Case $s = 2$. The nodes of the Gauss quadrature are $c_{1,2} = 1/2 \mp \sqrt{3}/6$. With $\ell_1(\tau) = (\tau - c_2)/(c_1 - c_2)$ and $\ell_2(\tau) = (\tau - c_1)/(c_2 - c_1)$ the method reads

$$\begin{aligned}
Y_1 &= y_0 + h \int_0^1 \left(\frac{1}{2}\, \ell_1(\sigma)\, B(Y_1) + \Big(\frac{1}{2} - \frac{\sqrt{3}}{3} \Big)\, \ell_2(\sigma)\, B(Y_2) \right) \nabla H(Y_\sigma)\, \mathrm{d}\sigma \\
Y_2 &= y_0 + h \int_0^1 \left(\Big(\frac{1}{2} + \frac{\sqrt{3}}{3} \Big)\, \ell_1(\sigma)\, B(Y_1) + \frac{1}{2}\, \ell_2(\sigma)\, B(Y_2) \right) \nabla H(Y_\sigma)\, \mathrm{d}\sigma \\
y_1 &= y_0 + h \int_0^1 \Big(\ell_1(\sigma)\, B(Y_1) + \ell_2(\sigma)\, B(Y_2) \Big) \nabla H(Y_\sigma)\, \mathrm{d}\sigma,
\end{aligned}$$

where Y_σ is the polynomial of degree 2 that interpolates the values y_0, Y_1, Y_2 at $t_0, t_0 + c_1 h, t_0 + c_2 h$, respectively. As we shall see in the next sections, this method exactly conserves the energy and quadratic Casimir functions, it is symmetric, of order 4, and it is invariant with respect to linear transformations.

3 Properties of the new class of integrators

The methods of the previous section have been designed to have exact energy preservation. It turns out that they have further interesting properties.

3.1 Exact energy preservation

Theorem 3.1 *If $B(y)$ is skew-symmetric for all y, then the numerical method of Definition 2.1 exactly preserves the energy, i.e., $H(y_n) = Const.$*

Proof From the fundamental theorem of calculus we have

$$H\big(u(t_0 + h)\big) - H\big(u(t_0)\big) \;=\; h \int_0^1 \nabla H\big(u(t_0 + \tau h)\big)^{\mathsf{T}}\, \dot{u}(t_0 + \tau h)\, \mathrm{d}\tau.$$

Replacing the derivative of $u(t)$ by (2.3) this expression becomes

$$\sum_{j=1}^{s} b_j \left(\int_0^1 \frac{\ell_j(\tau)}{b_j} \nabla H\big(u(t_0 + \tau h)\big)\, \mathrm{d}\tau \right)^{\mathsf{T}} B(Y_j) \int_0^1 \frac{\ell_j(\sigma)}{b_j}\, \nabla H\big(u(t_0 + \sigma h)\big)\, \mathrm{d}\sigma$$

which vanishes by the skew-symmetry of the matrix $B(y)$. □

3.2 Conservation of quadratic Casimir's

A function $C(y)$ is called a Casimir function of the differential equation (1.1) if $\nabla C(y)^{\mathsf{T}} B(y) = 0$ for all y. Along solutions of (1.1) we have $C\big(y(t)\big) = Const$, because $\frac{\mathrm{d}}{\mathrm{d}t} C\big(y(t)\big) = \nabla C\big(y(t)\big)^{\mathsf{T}} B\big(y(t)\big) \nabla H\big(y(t)\big) = 0$. This property is independent of the Hamiltonian $H(y)$.

Theorem 3.2 *Let $C(y) = y^{\mathsf{T}} A y$ (with a symmetric constant matrix A) be a Casimir function of the system (1.1). The energy preserving method based on the Gaussian quadrature formula of order $2s$ exactly preserves this Casimir.*

Proof Using again the fundamental theorem of calculus we have

$$C\big(u(t_0+h)\big) - C\big(u(t_0)\big) = h \int_0^1 \nabla C\big(u(t_0+\tau h)\big)^{\mathsf{T}} \dot{u}(t_0+\tau h)\,\mathrm{d}\tau.$$

Since the integrand is a polynomial of degree $2s-1$, an application of the Gaussian quadrature $(b_j, c_j)_{j=1}^s$ gives the exact result. The difference $C(y_1) - C(y_0)$ is thus equal to

$$h \sum_{j=1}^{s} b_j \nabla C\big(u(t_0+c_j h)\big)^{\mathsf{T}} B\big(u(t_0+c_j h)\big) \int_0^1 \frac{\ell_j(\tau)}{b_j} \nabla H\big(u(t_0+\tau h)\big)\,\mathrm{d}\tau,$$

which vanishes and proves the statement. □

The equations of motion for a free rigid body are a Lie-Poisson system with Casimir $C(y) = \|y\|_2^2$. The methods based on Gaussian quadrature thus preserve exactly the Hamiltonian and the Casimir.

3.3 Symmetry of the integrator

Theorem 3.3 *If the nodes c_i are symmetric, i.e., $c_{s+1-i} = 1 - c_i$, then the numerical method of Definition 2.1 is symmetric.*

Proof By the symmetry of the nodes we have $\ell_{s+1-i}(\tau) = \ell_i(1-\tau)$. This implies that the method, written as $y_1 = \Phi_h(y_0)$ satisfies $\Phi_{-h}(y) = \Phi_h^{-1}(y)$. □

3.4 Invariance with respect to linear transformations

A linear change of coordinates $z = Ty$ transforms a differential equation $\dot{y} = f(y)$ into $\dot{z} = \widehat{f}(z)$ with $\widehat{f}(z) = T f(T^{-1} z)$. A numerical method $\Phi_h^f(y_0)$ is called linear, if for any T we have

$$T \Phi_h^f(y_0) = \Phi_h^{\widehat{f}}(T y_0). \tag{3.1}$$

For the differential equation (1.1) the transformed problem is

$$\dot{z} = \widehat{B}(z) \nabla \widehat{H}(z), \quad z(t_0) = z_0 \tag{3.2}$$

with $\widehat{B}(z) = TB(T^{-1}z)T^{\mathsf{T}}$ and $\widehat{H}(z) = H(T^{-1}z)$. We call the integrator of Definition 2.1 linear, if (3.1) holds for $\widehat{f}(z) = \widehat{B}(z)\nabla\widehat{H}(z)$ with this special factorization of the vector field.[1]

[1] Since the numerical solution of our method depends on the factorization $B(y)\nabla H(y)$ of the vector field, it is important to fix the factorization in the definition of linearity. There is a slight abuse of notation by calling this weaker property still linear, but the same is done for partitioned linear multistep methods, where the partitioning of the system must also be fixed.

Theorem 3.4 *The integrator of Definition 2.1 is linear, i.e., if $\{y_n\}$ and $\{z_n\}$ are the numerical solutions corresponding to (1.1) and (3.2), respectively, and if $z_0 = Ty_0$, then we have $z_n = Ty_n$ for all n.*

Proof Only expressions of the form $B(y)\nabla H(\tilde{y})$ with possibly different y and $\tilde{y}$ are involved in the definition of the method. □

The differential equation (1.1) is said to have a linear symmetry T, if with $y(t)$ also $z(t) = Ty(t)$ is a solution. This is equivalent to $TB(T^{-1}z)\nabla H(T^{-1}z) = B(z)\nabla H(z)$, i.e., the transformed problem (3.2) is equal to the original one.

Corollary 3.1 *Assume that the problem (1.1) possesses a linear symmetry T that satisfies $TB(T^{-1}z)\nabla H(T^{-1}\tilde{z}) = B(z)\nabla H(\tilde{z})$ for all z and $\tilde{z}$. Then, the discrete flow of the method of Definition 2.1 has T as symmetry, i.e., if $\{y_n\}$ is a solution, then $\{Ty_n\}$ is also a solution.*

We remark that the condition on the linear symmetry in Corollary 3.1 is slightly weaker than what is called "linear special symmetry" in Proposition 3.8 of [8].

4 Discussion of the order

If the quadrature formula $(b_i, c_i)_{i=1}^s$ is of order $r = s + k$ ($0 \le k \le s$), then the order of the method of Definition 2.1 is at least $k+1$. This follows at once from $b_i^{-1} \int_0^1 \ell_i(\tau)\, \nabla H\big(u(t_0+\tau h)\big)\, \mathrm{d}\tau = H\big(u(t_0+c_i h)\big) + \mathscr{O}(h^{k+1})$, because the method is a perturbation of the classical collocation method. But what is the correct order? The answer can be obtained by interpreting the method as a partitioned Runge–Kutta method.

4.1 Extension of a theorem of Butcher

For a partitioned system of differential equations

$$\begin{aligned} \dot{y} &= f(y,z), \quad y(t_0) = y_0 \\ \dot{z} &= g(y,z), \quad z(t_0) = z_0 \end{aligned} \tag{4.1}$$

we consider methods that treat the y an z variables by different Runge–Kutta schemes. They are defined by (for $i = 1, \dots, s$)

$$\begin{aligned} Y_i &= y_0 + h\sum_{j=1}^s a_{ij} f(Y_j, Z_j) \qquad Z_i = z_0 + h\sum_{j=1}^s \widehat{a}_{ij} g(Y_j, Z_j) \\ y_1 &= y_0 + h\sum_{i=1}^s b_i f(Y_i, Z_i) \qquad z_1 = z_0 + h\sum_{i=1}^s \widehat{b}_i g(Y_i, Z_i). \end{aligned} \tag{4.2}$$

Order conditions, which are in one-to-one correspondence with bi-coloured rooted trees, are discussed in [6, Sect. II.15] and [5, Sect. III.2.2]. Elegant sufficient conditions for order p are based on simplifying assumptions. For convenience of notation,

we assume $\widehat{b}_i = b_i$ for all i, and we let $c_i = \sum_{j=1}^s a_{ij}$ and $\widehat{c}_i = \sum_{j=1}^s \widehat{a}_{ij}$. We then consider the conditions

$$B(\rho): \ \sum_{i=1}^s b_i c_i^{k-1} \widehat{c}_i^{\,l} = \frac{1}{k+l}, \qquad 1 \le k+l \le \rho$$
$$C(\eta): \ \sum_{i=1}^s a_{ij} c_j^{k-1} \widehat{c}_j^{\,l} = \frac{1}{k+l} c_i^{k+l}, \qquad 1 \le k+l \le \eta$$
$$D(\zeta): \ \sum_{i=1}^s b_i c_i^{k-1} \widehat{c}_i^{\,l} a_{ij} = \frac{b_j}{k+l}(1-\widehat{c}_j^{\,k+l}), \qquad 1 \le k+l \le \zeta$$

and we let $\widehat{C}(\eta), \widehat{D}(\zeta)$ be as $C(\eta), D(\zeta)$ with a_{ij} replaced by $\widehat{a}_{ij}$, and, only for $\widehat{C}(\eta)$, we replace also c_i in the right-hand side by $\widehat{c}_i$.

Theorem 4.1 *If a partitioned Runge–Kutta method (4.2) with $\widehat{b}_i = b_i$ for all i satisfies $B(\rho)$, $C(\eta)$, $\widehat{C}(\eta)$, $D(\zeta)$, $\widehat{D}(\zeta)$, then it is at least of order*

$$p = \min(\rho, 2\eta+2, \zeta+\eta+1).$$

The proof is the same as for (non-partitioned) Runge–Kutta methods (see [6, p. 208]). The only difference is that bi-coloured trees have to be considered instead of trees.

4.2 Interpreting the energy-preserving integrator as a partitioned RK-method

The energy-preserving integrator of Definition 2.1 treats the variable y in $B(y)$ and in $\nabla H(y)$ not in the same way. We therefore use different letters and put $Y_{i\tau} := Y_\tau$ and $Z_{i\tau} := Y_i$, so that formula (2.4) can be written as

$$\begin{aligned} Y_{i\tau} &= y_0 + h \sum_{j=1}^s \int_0^1 a_{i\tau,j\sigma} B(Z_{j\sigma}) \nabla H\big(Y_{j\sigma}\big) \,\mathrm{d}\sigma \\ Z_{i\tau} &= z_0 + h \sum_{j=1}^s \int_0^1 \widehat{a}_{i\tau,j\sigma} B(Z_{j\sigma}) \nabla H\big(Y_{j\sigma}\big) \,\mathrm{d}\sigma \end{aligned} \tag{4.3}$$

with $z_0 = y_0$ and

$$a_{i\tau,j\sigma} = \frac{\ell_j(\sigma)}{b_j} \int_0^\tau \ell_j(\alpha)\,\mathrm{d}\alpha, \qquad \widehat{a}_{i\tau,j\sigma} = \frac{\ell_j(\sigma)}{b_j} \int_0^{c_i} \ell_j(\alpha)\,\mathrm{d}\alpha. \tag{4.4}$$

For the numerical approximation after one step we get

$$\begin{aligned} y_1 &= y_0 + h \sum_{i=1}^s \int_0^1 b_{i\tau} B(Z_{i\tau}) \nabla H\big(Y_{i\tau}\big) \,\mathrm{d}\tau \\ z_1 &= z_0 + h \sum_{i=1}^s \int_0^1 \widehat{b}_{i\tau} B(Z_{i\tau}) \nabla H\big(Y_{i\tau}\big) \,\mathrm{d}\tau, \end{aligned} \tag{4.5}$$

where

$$b_{i\tau} = \widehat{b}_{i\tau} = \ell_i(\tau). \tag{4.6}$$

We notice that the formulas (4.3)-(4.5) constitute a partitioned Runge–Kutta method that has two particularities. First of all, it is consistent with the partitioned system of differential equations

$$\dot{y}=B(z)\nabla H(y), \quad y(t_0)=y_0$$
$$\dot{z}=B(z)\nabla H(y), \quad z(t_0)=z_0.$$

For $z_0=y_0$ we have $z(t)=y(t)$ for all t and both solution components are equal to the solution of (1.1). Secondly, we are concerned with a partitioned Runge–Kutta method having infinitely many stages. Whereas the stages are indexed by $i\in\{1,\dots,s\}$ in the method (4.2), they are indexed by $(i,\tau)\in\{1,\dots,s\}\times[0,1]$ in the method (4.3)-(4.5). A sum over i in (4.2) corresponds to a sum over i and an integral over τ in the method (4.3)-(4.5).

4.3 Verification of the simplifying assumptions

For the coefficients (4.4) we have, using $\sum_{j=1}^{s}\ell_j(\tau)=1$,

$$c_{i\tau}=\sum_{j=1}^{s}\int_0^1 a_{i\tau,j\sigma}\,\mathrm{d}\sigma=\tau, \qquad \widehat{c}_{i\tau}=\sum_{j=1}^{s}\int_0^1 \widehat{a}_{i\tau,j\sigma}\,\mathrm{d}\sigma=c_i. \tag{4.7}$$

We are now ready to check the simplifying assumptions.

Lemma 4.1 *Let $(b_i,c_i)_{i=1}^{s}$ represent a quadrature formula of order r. The coefficients (4.4), (4.6), and (4.7) then satisfy*

$$B(\rho):\ \sum_{i=1}^{s}\int_0^1 b_{i\tau}c_{i\tau}^{k-1}\widehat{c}_{i\tau}^{\,l}\,\mathrm{d}\tau=\frac{1}{k+l}, \qquad 1\le k+l\le\rho$$
$$C(\eta):\ \sum_{j=1}^{s}\int_0^1 a_{i\tau,j\sigma}c_{j\sigma}^{k-1}\widehat{c}_{j\sigma}^{\,l}\,\mathrm{d}\sigma=\frac{1}{k+l}c_{i\tau}^{k+l}, \qquad 1\le k+l\le\eta$$
$$\widehat{C}(\eta):\ \sum_{j=1}^{s}\int_0^1 \widehat{a}_{i\tau,j\sigma}c_{j\sigma}^{k-1}\widehat{c}_{j\sigma}^{\,l}\,\mathrm{d}\sigma=\frac{1}{k+l}\widehat{c}_{i\tau}^{\,k+l}, \qquad 1\le k+l\le\eta$$
$$D(\zeta):\ \sum_{i=1}^{s}\int_0^1 b_{i\tau}c_{i\tau}^{k-1}\widehat{c}_{i\tau}^{\,l}a_{i\tau,j\sigma}\,\mathrm{d}\tau=\frac{b_{j\sigma}}{k+l}(1-\widehat{c}_{j\sigma}^{\,k+l}), \qquad 1\le k+l\le\zeta$$
$$\widehat{D}(\zeta):\ \sum_{i=1}^{s}\int_0^1 b_{i\tau}c_{i\tau}^{k-1}\widehat{c}_{i\tau}^{\,l}\widehat{a}_{i\tau,j\sigma}\,\mathrm{d}\tau=\frac{b_{j\sigma}}{k+l}(1-\widehat{c}_{j\sigma}^{\,k+l}), \qquad 1\le k+l\le\zeta$$

with $\rho=r$, $\eta=\min(s,r-s+1)$, and $\zeta=\min(s-1,r-s)$.

Proof The proof is based on the identities $\int_0^1 g(\sigma)\mathrm{d}\sigma=\sum_{i=1}^{s}b_ig(c_i)$ for polynomials of degree $r-1$, and $\sum_{i=1}^{s}\ell_i(\tau)g(c_i)=g(\tau)$ for polynomials of degree $s-1$. We present details for the simplifying assumption $D(\zeta)$. The other conditions are proved in a similar way.

Inserting the expressions (4.4), (4.6) and (4.7) into the left-hand side of condition $D(\zeta)$ and using $\sum_{i=1}^{s} \ell_i(\tau)\, c_i^l = \tau^l$ for $0 \le l \le s-1$ yields

$$\sum_{i=1}^{s} \int_0^1 \ell_i(\tau)\, \tau^{k-1}\, c_i^l\, \frac{\ell_j(\sigma)}{b_j} \int_0^\tau \ell_j(\alpha)\, \mathrm{d}\alpha\, \mathrm{d}\tau = \int_0^1 \tau^{k+l-1}\, \frac{\ell_j(\sigma)}{b_j} \int_0^\tau \ell_j(\alpha)\, \mathrm{d}\alpha\, \mathrm{d}\tau.$$

Partial integration then shows that this expression equals

$$\ldots = \frac{\ell_j(\sigma)}{b_j} \left(\frac{\tau^{k+l}}{k+l} \int_0^\tau \ell_j(\alpha)\, \mathrm{d}\alpha \Big|_{\tau=0}^{\tau=1} - \int_0^1 \frac{\tau^{k+l}}{k+l}\, \ell_j(\tau)\, \mathrm{d}\tau \right) = \frac{\ell_j(\sigma)}{k+l} \left(1 - c_j^{k+l} \right),$$

which corresponds to the right-hand side of $D(\zeta)$. In the last equality we have replaced the integral over τ by the quadrature formula, which does not introduce an error when $k+l+s \le r$. Since $k \ge 1$, the simplifying assumption $D(\zeta)$ thus holds with $\zeta = \min(s-1, r-s)$. □

Standard limit considerations show that Theorem 4.1 is also valid for partitioned Runge–Kutta methods with a continuum of stages. We therefore have proved the following result.

Theorem 4.2 *Let $(b_i, c_i)_{i=1}^{s}$ represent a quadrature formula of order r. The energy-preserving integrator of Definition 2.1 has order*

$$p = \min(r, 2r - 2s + 2).$$

For methods based on Gaussian quadrature we have order $p = 2s$. An order reduction (compared to classical collocation methods) occurs only for $r < 2s-2$.

5 Numerical experiments

After having shown many nice and important features for the new class of energy-preserving integrators, it is natural to investigate the question to which extent the proposed methods are close to Poisson integrators. It is obvious that they cannot conserve the Hamiltonian and the Poisson structure at the same time, because this is not possible for the special case of canonical Hamiltonian systems (see [1]). But, is it possible that our energy-preserving integrators are conjugate to a Poisson integrator? This would imply that all Casimir functions are nearly conserved without drift.

To study this question, we consider a Lotka–Volterra system [3], for which

$$B(y) = \begin{pmatrix} 0 & cy_1y_2 & bcy_1y_3 \\ -cy_1y_2 & 0 & -y_2y_3 \\ -bcy_1y_3 & y_2y_3 & 0 \end{pmatrix}, \quad H(y) = aby_1 + y_2 - ay_3 + \nu \ln y_2 - \mu \ln y_3,$$

and where the parameters satisfy $abc = -1$. The corresponding Poisson system possesses the Casimir

$$C(y) = ab \ln y_1 - b \ln y_2 + \ln y_3.$$

For our experiment we have chosen as parameters $a = -2$, $b = -1$, $c = -0.5$, $\nu = 1$, $\mu = 2$, and initial values $y(0) = (1.0, 1.9, 0.5)$. With these data the solution is periodic.

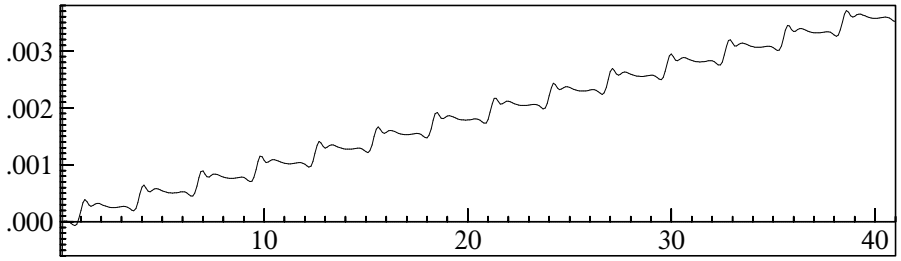

Fig. 5.1 Time evolution of the error in the Casimir function along the numerical solution of the fourth order energy-preserving method based on Gauss points.

To this problem we apply the fourth order integrator of Section 2.3 with step size $h = 0.1$. By construction, the Hamiltonian $H(y)$ is preserved up to round-off along the numerical solution. However, the error in the Casimir function $C(y)$ shows a linear drift of size $\mathcal{O}(th^4)$, see Figure 5.1. This demonstrates that the integrator is not conjugate to a Poisson integrator.

6 Conclusion

In this work we propose a new class of energy-preserving integrators for Hamiltonian systems with non-canonical structure matrix. The methods conserve also quadratic Casimir functions and they are of arbitrarily high order. In contrast to previously proposed energy-preserving methods, our methods are invariant with respect to linear transformations.

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