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A new class of energy-preserving numerical integration methods

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Abstract
The first ever energy-preserving B-series numerical integration method for (ordinary) differential equations is presented and applied to several Hamiltonian systems. Related novel Lie algebraic results are also discussed.

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1. Introduction

In recent years, geometric numerical integration methods have come to the fore, partly as an alternative to traditional methods such as Runge–Kutta methods.

A numerical method is called *geometric* if it preserves one or more physical/geometric properties of the system exactly (i.e. up to round-off error). Examples of such geometric properties that can be preserved are (first) integrals, symplectic structure, symmetries and reversing symmetries, phase–space volume, Lyapunov functions, foliations, etc. Geometric methods have applications in many areas of physics, including celestial mechanics, particle accelerators, molecular dynamics, fluid dynamics, pattern formation, plasma physics, reaction-diffusion equations, and meteorology. Recent surveys of this field have been given in [9, 12, 14, 18].

This paper will be concerned with the preservation of energy (cf [7]), a crucial property of mechanical systems. Let us therefore first review the status quo with respect to the preservation of first integrals more generally. An ordinary differential equation

$$\frac{\mathrm{d}x}{\mathrm{d}t} = f(x), \qquad x \in \mathbb{R}^n. \tag{1}$$

possesses the first integral $I(x)$ if $f(x) \cdot \nabla I(x) = 0$. In [16] it was shown that (under some mild technical conditions) $f(x) \cdot \nabla I(x) = 0$ if and only if there exists a skew-symmetric matrix $S(x)$ such that

$$f(x) = S(x)\nabla I(x). \tag{2}$$

This result was used in [15, 16] to construct general integral-preserving integration methods using the so-called discrete gradients. The most prominent alternative methods to preserve integrals are projection methods [9]. Drawbacks of both these classes of algorithms are that they require the input of the functional form of the integral to be conserved, and that they are not linearly covariant [17].

2. Energy-preserving numerical integration methods

In this paper, we describe a novel class of B-series methods (this term will be explained below) that preserves energy for all (canonical) Hamiltonian vector fields. Moreover, this class of methods is user friendly in the sense that the user is not required to input the energy function, or even be aware that the system preserves energy. The methods require only knowledge of the vector field itself (a necesssary input for all integration methods), i.e. when we are integrating the ordinary differential equation (1) we require the vector field f. The prototype of this novel class of energy-preserving B-series methods is the following method, which we call an 'averaged vector field method':

$$\frac{x_{n+1} - x_n}{h} = \int_0^1 f((1-\xi)x_n + \xi x_{n+1})\,\mathrm{d}\xi, \tag{3}$$

where here and below h denotes the time step of the method.

To show that the method (3) preserves energy, we proceed as follows: first substitute

$$f(x) = S\nabla H(x) \tag{4}$$

in (3). Here S denotes an arbitrary *constant* skew-symmetric matrix and H denotes the (Hamiltonian) energy function. This substitution yields

$$\frac{x_{n+1} - x_n}{h} = S\int_0^1 \nabla H((1-\xi)x_n + \xi x_{n+1})\,\mathrm{d}\xi. \tag{5}$$

Now take the scalar product with $\int_0^1 \nabla H\,((1-\xi)x_n + \xi x_{n+1})\,\mathrm{d}\xi$ on both sides of the equation, yielding

$$\frac{1}{h}\int_0^1 (x_{n+1} - x_n)\cdot\nabla H((1-\xi)x_n + \xi x_{n+1})\,\mathrm{d}\xi = 0, \tag{6}$$

i.e.

$$\frac{1}{h}\int_0^1 \frac{\mathrm{d}}{\mathrm{d}\xi} H((1-\xi)x_n + \xi x_{n+1})\,\mathrm{d}\xi = 0 \tag{7}$$

which, using the Fundamental Theorem of Calculus, yields

$$\frac{1}{h}(H(x_{n+1}) - H(x_n)) = 0. \tag{8}$$

It follows that the energy H is conserved at every time step, provided the vector field has the form (4). (Note that we do not require the constant matrix S to be invertible. Hence our methods also apply to Poisson systems with constant Poisson structures.)

3. Numerical results

The integrator (3) was applied to the double well and Hénon–Heiles systems, with respective Hamiltonian functions

$$H(q, p) = \tfrac{1}{2}p^2 + \tfrac{1}{2}(q^2 - 1)^2 \tag{9}$$

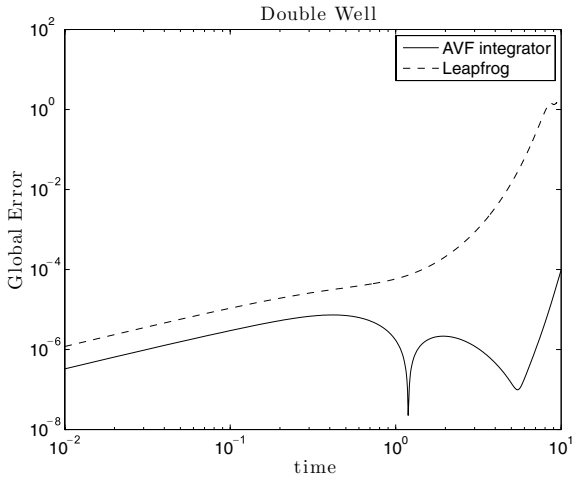


Figure 1. Double well system: global errors incurred using the averaged vector field (solid line) and leapfrog (dashed line) integrators. With initial condition $q = -1$, $p = 1.000\,001$ the initial energy is marginally larger than the critical value $E_c = \frac{1}{2}$. The step size was $h = 0.01$ and $t_{\max} = 10$.

for the double well system, and

$$H(q_1, q_2, p_1, p_2) = \tfrac{1}{2}\left(q_1^2 + q_2^2 + p_1^2 + p_2^2\right) + q_1^2 q_2 - \tfrac{1}{3}q_2^3 \tag{10}$$

for Hénon–Heiles. The equations of motion are as determined by the canonical matrix $S = \left(\begin{smallmatrix} 0 & Id \\ -Id & 0 \end{smallmatrix}\right)$ in both cases [13]. Both systems have a critical energy value E_c at which the qualitative nature of their solutions changes—for the double well $\left(E_c = \frac{1}{2}\right)$ from oscillations around one potential minimum to an orbit that encloses both, and for Hénon–Heiles $\left(E_c = \frac{1}{6}\right)$ from bounded to unbounded orbits. In the experiments shown here, for the double well the initial energy was slightly larger than E_c, and for Hénon–Heiles it was exactly E_c with initial spatial coordinates (q_1, q_2) at a point on the boundary of the critical triangular region (see [13]) shown in figure 2. For comparisons we also solve these two systems using a second-order symplectic method, the leapfrog method [9].

For the double well system, both integrators exhibit the correct qualitative behaviour, but the leapfrog error (figure 1) grows rapidly to values approximating the maximum diameter of the phase-plane orbit. For Hénon–Heiles the averaged vector field integrator (figure 2, left) stays within the stable zone, whilst leapfrog (figure 2, right) strays outside and soon becomes completely unstable.

4. Energy-preserving linear combinations of rooted trees

The importance of algebras of trees in quantum field theory has recently become apparent (cf e.g. [3]). The connection between the algebras in the field theory and those in numerical integration was pointed out in [1]. Here we will explore the algebraic implications of our novel class of energy-preserving integrators.

For any approximate solution

$$x_{n+1} = \phi_h(x_n) \tag{11}$$

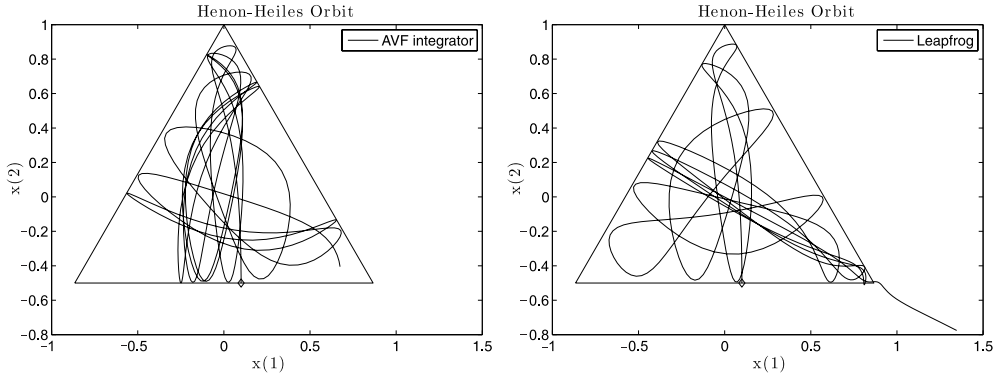


Figure 2. Hénon–Heiles system: configuration space orbits obtained using the averaged vector field (left-hand plot) and leapfrog (right-hand plot) integrators. The initial point (marked) on the lower edge of the triangle at $q_1 = 0.1$, $q_2 = -0.5$, $p_1 = p_2 = 0$ corresponds to the critical energy value $E_c = \frac{1}{6}$. The step size was $h = 0.16$ and $t_{\max} = 71$.

of any differential equation $\mathrm{d}x/\mathrm{d}t = f(x)$, one can introduce the so-called modified vector field $\mathrm{d}x/\mathrm{d}t = \tilde{f}_{(h)}(x)$ for which formally (11) provides the exact solution, i.e. $\phi_h = \mathrm{e}^{h\tilde{f}_{(h)}\frac{\partial}{\partial x}}$. The advantage of geometric integration methods is that, loosely speaking, their modified vector fields belong to the same class as the original vector fields one wishes to integrate. That is, modified vector fields of symplectic methods are Hamiltonian, modified vector fields of volume-preserving methods are divergence-free, modified vector fields of integral-preserving methods preserve the original integral, etc [8]. Motivated by this connection we have determined the modified vector field for our averaged vector field method (3). Its ith component is given by

$$\tilde{f}^i_{(h)} = f^i + \tfrac{1}{12}h^2 f^i_j f^j_k f^k + O(h^4)\ldots \tag{12}$$

where subscripts denote partial derivatives $\left(\text{i.e. } f^i_j = \frac{\partial f^i}{\partial x^j}\right)$, and repeated indices imply summation. Products such as $f^i_j f^j_k f^k$ are called *elementary differentials*[3]. Closer inspection reveals the basis of energy-preserving linear combinations of elementary differentials. This is illustrated in table 1, where the results are given up to order 5.

Here we have used the standard representation of elementary differentials by rooted trees [2, 10]. For example,  denotes $f^i_j f^j_{kl} f^k f^l$. The fact that, e.g. the fourth-order combination in table 1 is energy preserving can be shown as follows:

$$f^i_j f^j_{kl} f^k f^l + f^i_{jk} f^j f^k_l f^l = \tilde{S}(x)\nabla H(x), \tag{13}$$

where (in accordance with (2)) $\tilde{S}(x)$ is a skew-symmetric matrix. It is given by

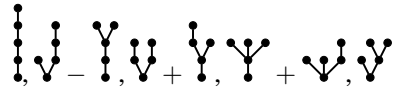
$$\tilde{S} = S\mathcal{H}ST S + ST S\mathcal{H}S, \tag{14}$$

with the symmetric matrices $\mathcal{H}(x)$ and $T(x)$ being given by

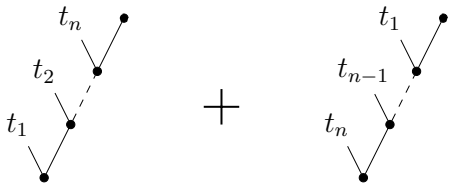
$$\mathcal{H}_{ij} := \frac{\partial^2 H}{\partial x_i \partial x_j}, \qquad \text{and} \qquad T_{ij} := \frac{\partial^3 H}{\partial x_i \partial x_j \partial x_k} S^{kl} \frac{\partial H}{\partial x_l}. \tag{15}$$

[3] B-series methods may be defined as those methods whose modified vector fields can (formally) be expanded in terms of elementary differentials.

Table 1. Energy-preserving linear combinations of rooted trees (elementary differentials), up to fifth order.

Order	Energy-preserving linear combinations
1	
2	–
3	
4	
5	

More generally, energy-preserving linear combinations of rooted trees/elementary differentials are given by



when n is even, and

when n is odd, where $t_1, t_2, \ldots, t_n$ are arbitrary trees. The set of all energy-preserving linear combinations of rooted trees/elementary differentials forms a large Lie sub-algebra of the Lie algebra of all rooted trees/elementary differentials.

5. Discussion

- After we discovered these new energy-preserving methods, we found that, in [5], Faou *et al* have derived the conditions a B-series method must satisfy in order to be energy-preserving (cf also [4]). However it seems that until now no actual method had been found that satisfies the derived conditions.
- Space limitations prevent us exhibiting our entire new class of energy-preserving B-series methods here [4]. We restrict ourselves to exhibiting the following simple (energy-preserving) generalization of the method (3):

$$\frac{x_{n+1} - x_n}{h} = \left(\delta^i_j + \alpha h^2 f^i_k(\hat{x}) f^k_j(\hat{x})\right) \int_0^1 f^j\left((1-\xi)x_n + \xi x_{n+1}\right) \mathrm{d}\xi, \quad (16)$$

where α is an arbitrary constant, δ^i_j is the Kronecker delta, and we can take e.g. $\hat{x} = x_n$ or $\hat{x} = \frac{x_n + x_{n+1}}{2}$.

[4] We hope to expand on the contents of this paper in a forthcoming publication.

For $\alpha = 0$ we recover the second-order method (3). For $\alpha = -\frac{1}{12}$ and $\hat{x} = x_n$ the method is third order. For $\alpha = -\frac{1}{12}$ and $\hat{x} = \frac{x_n + x_{n+1}}{2}$ the method is of fourth order accuracy.

- An unusual feature of the methods given in this paper (both methods (3) as well as (16)) is that they require anti-derivatives (i.e. definite integrals) of the vector field. Such a feature is not entirely novel. Something similar is required in general volume-preserving integrators. For vector fields where these anti-derivatives are available in a closed form (such as polynomial vector fields) this of course presents no barrier. The general case awaits further investigation.
- The B-series methods presented in this paper share the advantageous properties common to all B-series methods [19]. For example, they preserve all linear integrals and foliations, all affine symmetries, and are covariant with respect to all affine transformations. In addition, those methods that are self-adjoint preserve all affine reversing symmetries.
- It has been proven that, in general, there can exist no numerical integration method that preserves both the symplectic structure as well as the energy of a Hamiltonian system [6]. Therefore for a given problem, one must make a choice. Much can be said about the advantages and disadvantages of either choice, cf e.g. [20]. In general we expect energy-preservation to be more important in lower dimensions than in higher dimensions, and particularly for compact level sets, and even more particularly close to critical level sets. An advantage of symplectic integrators is their preservation of quasi-periodic orbits. For Hamiltonian systems with (affine) time-reversal symmetry, this may also be achieved by self-adjoint energy-preserving methods such as (3).
- Note that we do not claim that our methods preserve integrals of arbitrary differential equations [4]. Our methods preserve the integral only for those systems (2) where the skew-symmetric matrix S is constant.
- It can be shown that the ratio of the dimension of the space of n^{th}-order energy-preserving linear combinations of rooted trees to the dimension of the space of n^{th}-order rooted trees approaches 1 as n approaches ∞.

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References

[1] Brouder Ch 2000 Runge–Kutta methods and renormalization *Euro. Phys. J.* C **12** 521–34
[2] Butcher J C 1987 *The Numerical Analysis of Ordinary Differential Equations. Runge–Kutta and General Linear Methods* (New York: Wiley)
[3] Connes A and Kreimer D 1998 Hopf algebras, renormalization and noncommutative geometry *Commun. Math. Phys.* **199** 203–45
[4] Chartier P, Faou E and Murua A 2006 An algebraic approach to invariant-preserving integrators: the case of quadratic and Hamiltonian invariants *Numer. Math.* **103** 575–90
[5] Faou E, Hairer E and Pham T-L 2004 Energy conservation with non-symplectic methods: examples and counter-examples *BIT* **44** 699–709
[6] Ge Z and Marsden J E 1988 Lie–Poisson Hamilton–Jacobi theory and Lie–Poisson integration *Phys. Lett.* A **133** 134–9
[7] Greenspan D 2006 *Numerical Solution of Ordinary Differential Equations for Classical, Relativistic and Nano Systems* (New York: Wiley)
[8] Hairer E 1994 Backward analysis of numerical integrators and symplectic methods *Ann. Numer. Math.* **1** 107–32

[9] Hairer E, Lubich C and Wanner G 2002 Geometric numerical integration *(Springer Series in Computational Mathematics* vol 31) (Berlin: Springer)
[10] Hairer E, Norsett S P and Wanner G 1993 Solving ordinary differential equations: I. Nonstiff problems 2nd edn *(Springer Series in Computational Mathematics* vol 8) (Berlin: Springer)
[11] Iserles A and Zanna A 2000 Preserving algebraic invariants with Runge–Kutta methods *J. Comput. Appl. Maths* **125** 69–81
[12] Leimkuhler B and Reich S 2004 *Simulating Hamiltonian Dynamics, Cambridge Monographs on Applied and Computational Mathematics* (Cambridge: Cambridge University Press)
[13] Lichtenberg A J and Liebermann M A 1992 *Regular and Chaotic Dynamics* 2nd edn (New York: Springer)
[14] McLachlan R I and Quispel G R W 2002 Splitting methods *Acta Numer.* **11** 341–434
[15] McLachlan R I, Quispel G R W and Robidoux N 1998 Unified approach to Hamiltonian systems, Poisson systems, Gradient systems, and systems with Lyapunov functions or first Integrals *Phys. Rev. Lett.* **81** 2399–403
[16] McLachlan R I, Quispel G R W and Robidoux N 1999 Geometric integration using discrete gradients *Phil. Trans. R. Soc.* A **357** 1021–45
[17] McLachlan R I, Quispel G R W and Turner G S 1998 Numerical integrators that preserve symmetries and reversing symmetries *SIAM J. Numer. Anal.* **35** 586–99
[18] Quispel G R W and McLachlan R I (eds) 2006 Special issue on geometric numerical integration of differential equations *J. Phys. A: Math. Gen.* **39** 5251–651
[19] Tse P S P 2007 Geometric Numerical Integration *Ph.D. Thesis* La Trobe University
[20] Simo J C, Tarnow N and Wong K K 1992 Exact energy-momentum conserving algorithms and symplectic schemes for nonlinear dynamics *Comput. Methods Appl. Mech. Eng.* **100** 63–116