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ENERGY-PRESERVING METHODS AND B-SERIES

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Summary. We consider energy-preservation for Runge-Kutta methods and B-series methods, propose new energy-preserving methods and investigate the importance of energy preservation (in symmetric integration methods) versus the preservation of symplecticity.

1 INTRODUCTION

Given the system of ordinary differential equations (ODEs)

$$\dot{y} = f(y), \quad y(0) = y_0 \in \mathbf{R}^n,$$

assume $H : \mathbf{R}^n \to \mathbf{R}$ is an invariant or the energy of the system, and that we have $f(y) = S\,\nabla H(y)$ with S an $n \times n$, skew-symmetric matrix[1].

To derive energy-preserving numerical integration methods for these problems one can use discrete gradient techniques, [5], [7]. Such methods rely on appropriate approximations of $\nabla H(y)$ and S (in the case S depends on y), and in general can not be expanded in a B-series. (i.e. they are not so called B-series methods).

A B-series for the system $\dot{y} = f(y)$ is a formal series in powers of the step size h and in terms

[1] This implies that the energy H is preserved along the solution of the ODE, that is

$$\frac{dH(y(t))}{dt} = \nabla H(y)^T \cdot f(y) = \nabla H(y)^T \cdot S\,\nabla H(y) = 0.$$

of elementary differentials [6],

$$\begin{aligned} B(a,y) &= y + \sum_{\tau\in\mathcal{T}} \frac{h^{|\tau|}}{\sigma(\tau)} a(\tau)F(\tau)(y) \\ &= y + ha(\bullet)f(y) + h^2 a([\bullet])f'f(y) + h^3 a([\bullet,\bullet])f''(f,f)(y) + \cdots \end{aligned}$$

Rooted trees are defined recursively and the set of rooted trees is $\mathcal{T} := \{\bullet, [\bullet], [\bullet,\bullet], [[\bullet]], \cdots\}$, $|\tau|$ is the number of nodes of the tree τ, $\sigma(\tau)$ is the symmetry of the tree, $F(\tau)$ is the elementary differential associated to τ and we have

$F(\bullet) = f, \quad F([\bullet]) = f'f, \quad F([\bullet,\bullet]) = f''(f,f), \quad F([[\bullet]]) = f'f'f, \quad \ldots$

Faou, Hairer and Pham [4], and Chartier, Faou and Murua [1], characterized all energy preserving B-series for Hamiltonian problems ($\dot{y} = S\,\nabla H(y)$, with S the canonical symplectic matrix). Consider the linear space obtained by taking linear combinations of elements of $\mathcal{T}$ and consider the linear subspaces generated by all the rooted trees of order n. In [3] we characterize the linear combinations of trees with n nodes corresponding to energy-preserving vector fields, find their annihilator and their dimensions.

2 Energy-preserving B-series methods of high order

An example of a numerical integrator which is not a Runge-Kutta method and which admits a B-series expansion is the average vector field (AVF) method, namely

$$y_{n+1} - y_n = h\int_0^1 f((1-\xi)y_n + \xi y_{n+1})\,d\xi, \quad y_n \approx y(t_n),\ n = 0,1,\ldots. \tag{1}$$

Under the assumption that S is a constant matrix, this is a discrete gradient method, as recently observed by Quispel and McLaren [8].

An extension of this method to a class of higher order energy-preserving methods is

$$f[Y_{i-1}, Y_i] := \int_0^1 f(Y_{i-1}\xi + Y_i(1-\xi))\,d\xi,$$

$$Y_i = Y_{i-1} + \beta_i h \left(I + h^2 \sum_{j=1}^{s} a_{i,j} f'\left(\frac{Y_{j-1}+Y_j}{2}\right)^2 \right) f[Y_{i-1}, Y_i] \tag{2}$$

$i = 1,\ldots,s$ $Y_0 = y_n$ $y_{n+1} := Y_s$, where f' is the Jacobian of f, [2].

Alternatively one can take $(\int_0^1 f(Y_{i-1}\xi + Y_i(1-\xi))\,d\xi)^2$ instead of $f'((Y_{j-1}+Y_j)/2)^2$.

3 Time-symmetry and numerical experiments

Recall that a one step method $y_{n+1} = \phi_h(y_n)$ is time-symmetric if it is such that $y_n = \phi_{-h}(y_{n+1})$ when applied to a reversible system (e.g. an Hamiltonian system). All the methods considered in the previous section are time-symmetric.

We consider the performance of classical time-symmetric and symplectic Runge-Kutta methods to a problem with a non-polynomial Hamiltonian function, and we compare them to the energy-preserving time-symmetric methods presented in the previous section. The methods we

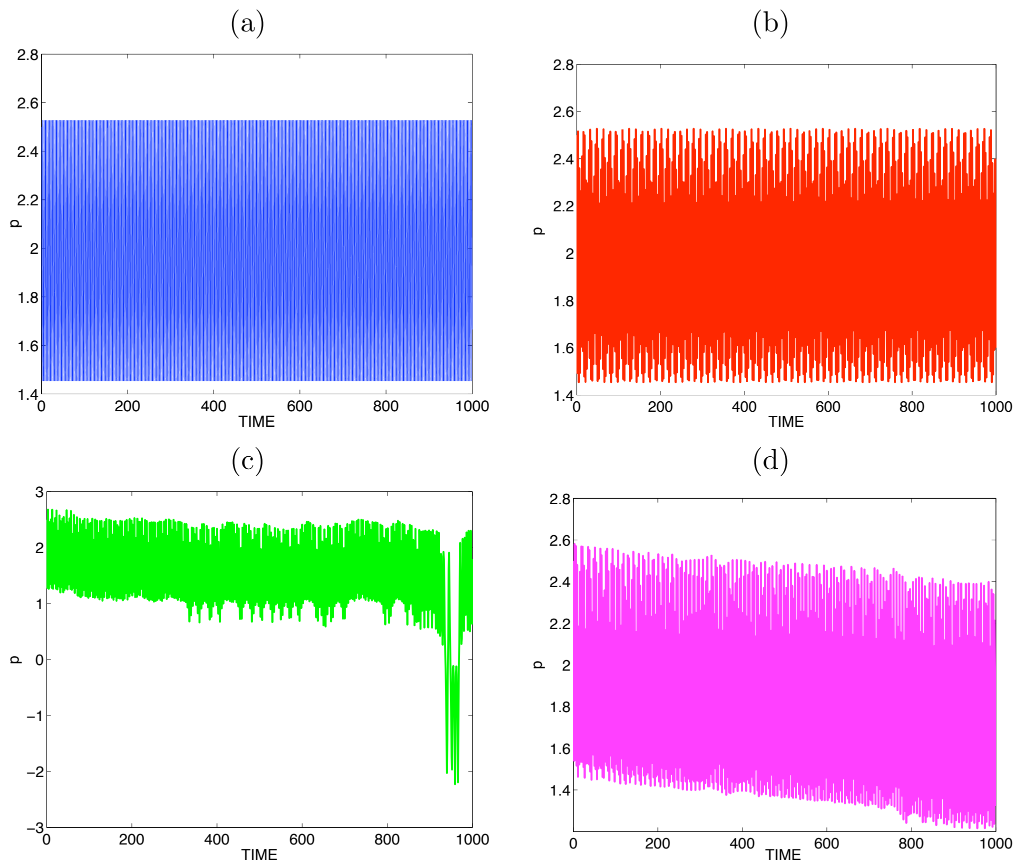

Figure 1: Momentum on the interval $[0, 1000]$. (a) The exact solution computed in Matlab with ode15s, at low tolerance, the integration requires 92577 setps. (b) Time-symmetric energy-preserving method of order 4 (avf4). (c) Implicit midpoint (symplectic of order 2). (d) Lobatto III B order 4, implicit and time-symmetric.

used are the Lobatto III B of order 4 (time-symmetric), the implicit midpoint rule (symplectic and of order 2) and the avf method of order 4 from the previous section.

The Hamiltonian function is $H = \frac{1}{2}p^2 - \cos(q) + \frac{1}{5}\sin(2q)$, this test case was considered also in [4]. In figure 1 we plot the momentum variable at $T = 1000$, using the (rather large) step-size of integration $h = 1$ for all the methods.

In figure 2 we consider the energy value along the numerical solution.

In this test problem the avf4 performs better than the time-symmetric Lobatto III B method of the same order but more surprisingly also better of the symplectic method.

4 Conclusions

The aim of this project is to contribute to the understanding of how the linear space generated by the set of rooted trees divide into subspaces corresponding to energy-preserving vector fields. We also present a class of energy-preserving high order B-series methods and test them on an Hamiltonian problem, showing that sometime a time symmetric energy-preserving method

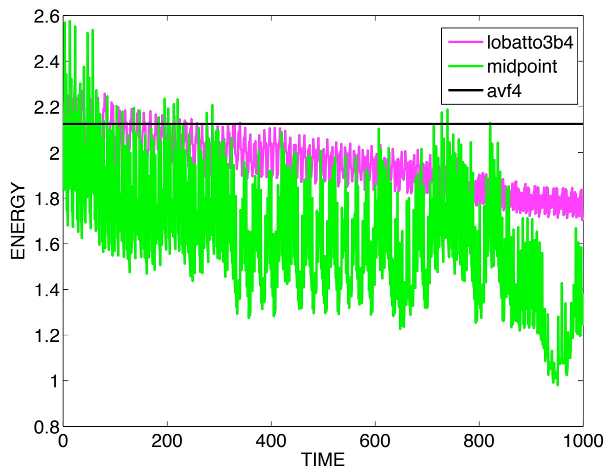

Figure 2: Energy versus time

might perform even better than a symplectic method.

REFERENCES

[1] Chartier, P. and Faou, E. and Murua, A, *An algebraic approach to invariant preserving integrators: the case of quadratic and Hamiltonian invariants*, Num. Math. 2006.

[2] E. Celledoni, D. McLaren, R.I. McLachlan, B. Owren, G.R. Quispel, W. Wright, *Energy-preserving Runge–Kutta methods*, submitted to M2AN (Mathematical Modelling and Numerical Analysis).

[3] E. Celledoni, D. McLaren, R.I. McLachlan, B. Owren, G.R. Quispel, W. Wright, *Energy-preserving B-series methods*, in preparation.

[4] Faou, E. and Hairer, E. and Pham, T. L., *Energy conservation with non-symplectic methods: examples and counter-examples*, BIT, 2004.

[5] Gonzalez, O., *Time integration and discrete Hamiltonian systems*, J. Nonlinear Sci., 1996.

[6] E. Hairer and G. Wanner *Solving ordinary differential equations. II*, Springer Verlag, (1993).

[7] McLachlan, R. I. and Quispel, G. R. W. and Robidoux, N., *Geometric integration using discrete gradients*, J. R. Soc. Lond. Philos. Trans. Ser. A Math. Phys. Eng. Sci., 1999.

[8] G. R. W. Quispel and D. I. McLaren *A new class of energy-preserving numerical integration methods*, J. Phys. A, 2008.