GEOMETRIC INTEGRATION BY PLAYING WITH MATRICES

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Dedicated to the 70^{th} birthday of Gerhard Wanner

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1 - Overview

- Geometric Integration
- some history
- geometric Runge-Kutta methods
- matrix formulation of the methods
- generalized W-transform
- energy-conservation (and some generalizations)
- symplecticity
- both of them, too ...
- concluding remarks

2 - Conservative problems

We shall deal with problems in the form

$$y'(t) = f(y(t)), \qquad y(0) = y_0 \in \mathbb{R}^m,$$

for which there exists

$$L : \mathbb{R}^m \longrightarrow \mathbb{R}^\nu$$

such that

$$L(y(t)) = L(y_0), \qquad t \geq 0.$$

That is, the dynamical system admits ν constants of motion.

3 - Geometric Integration

The numerical solution of conservative problems is an active field of investigation:

- the numerical methods induce a corresponding discrete vector field;
- it is desirable that the latter is able to reproduce geometrical properties of the continuous one.

Because of this reason, it has become customary to refer this field of investigation to as geometric integration.

4 - An Old Story ...

Conceptually, geometric integration:

- can be led back to the early work of G. Dahlquist on differential equations, about 50 years ago,
- his aim being to reproduce the asymptotic stability of equilibria for the trajectories produced by the numerical methods,
- thus resulting in the well-known linear stability analysis of the methods.

5 - Hamiltonian Problems

In particular, we shall deal with the numerical solution of Hamiltonian problems, which are encountered in many real-life applications, ranging from the nano-scale of molecular dynamics, to the macro-scale of celestial mechanics:

$$y' = J\nabla H(y), \qquad y(0) = y_0 \in \mathbb{R}^{2m}, \qquad J = \begin{pmatrix} & I_m \\ -I_m & \end{pmatrix},$$

where $J^T = -J = J^{-1}$. The scalar function $H(y)$ is the Hamiltonian of the problem and its value is constant during the motion, namely

$$H(y(t)) \equiv H(y_0), \qquad \forall t \geq 0,$$

since

$$\frac{\mathrm{d}}{\mathrm{d}t} H(y(t)) = \nabla H(y(t))^T y'(t) = \nabla H(y(t))^T J \nabla H(y(t)) = 0.$$

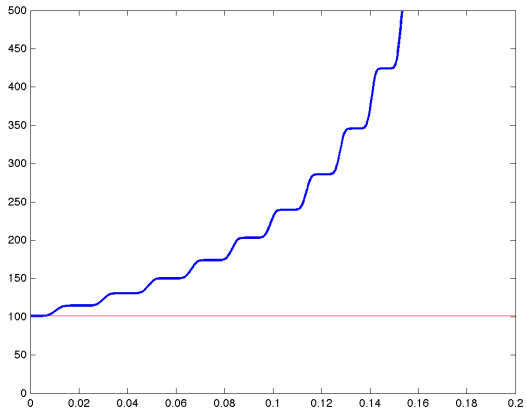
6 - Energy conservation

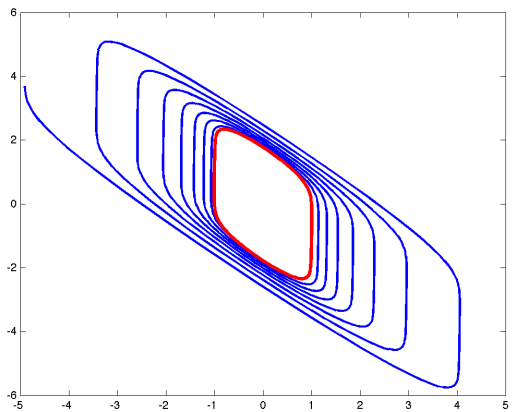
Often, the Hamiltonian H is also called the energy, since for isolated mechanical systems it has the physical meaning of total energy.

Consequently, energy conservation is an important feature in the simulation of such problems.

"Usual" numerical methods often exhibit a drift in the energy.

This, in turn, hinders the possibility of performing correct long-term simulations.





7 - Symplecticity of the map

The continuous map associated with the Hamiltonian problem,

$$\phi_t : y_0 \to y(t),$$

can be proved to be symplectic. That is, by setting ϕ'_t the Jacobian of ϕ_t, then

$$(\phi'_t)^T J(\phi'_t) = J.$$

The conservation of the Hamiltonian can be proved to derive from the symplecticity of the map, via an infinite number of infinitesimal contact transformations (see, e.g., [1]).

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[1] H. Goldstein, C.P. Poole, J.L. Safko. *Classical Mechanics*, Addison Wesley, 2001.

8 - Symplectic methods

A rough idea about symplectic methods can be found in early work of Gröbner [2]. Symplectic Runge–Kutta methods have been then studied by Feng Kang [3], Sanz-Serna [4], and Suris [5].

Such methods are obtained by imposing that the discrete map, associated with a given numerical method, is symplectic, as is the continuous one.

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[2] W. Gröbner. *Gruppi, Anelli ed Algebre di Lie*. Edizioni Cremonese, Rome, 1975.

[3] Feng Kang. On Difference Schemes and Symplectic Geometry. *Science Press, Beijing*, 1985.

[4] J.M. Sanz-Serna. Runge-Kutta schemes for Hamiltonian systems. *BIT* 28 (1988) 877-883.

[5] Y.B. Suris. The canonicity of mappings generated by Runge-Kutta type methods when integrating the systems $x'' = -\partial U/\partial x$. *U.S.S.R. Comput. Math. and Math. Phys.* 29 (1989) 138–144.

9 - Backward error analysis

Symplectic methods usually perform much better than standard ones.

Since for the continuous map symplecticity implies energy-conservation, then one expects that something similar happens for the discrete map as well.

As a matter of fact, under suitable assumptions, it can be proved that, when a symplectic method is used with a constant step-size h, then the numerical solution satisfies a perturbed Hamiltonian problem [6],

$$\tilde{y}' = J\nabla \tilde{H}_h(\tilde{y}), \qquad \tilde{y}(0) = y_0 \in \mathbb{R}^{2m}.$$

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[6] G. Benettin, A. Giorgilli. On the Hamiltonian interpolation of near to the identity symplectic mappings with application to symplectic integration algorithms. *J. Statist. Phys.* 74 (1994) 1117-1143.

10 - Energy conservation

The previous result then provides a quasi-conservation property of the Hamiltonian over "exponentially long times" . (See also the comprehensive monograph [7]).

Even though this is an interesting feature, nonetheless, it constitutes a somewhat weak stability result since, in general,

- it doesn't extend to infinite intervals,
- cannot avoid severe restrictions on the stepsize,

as a classical stability analysis would require.

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[7] E. Hairer, C. Lubich, G. Wanner, *Geometric Numerical Integration, 2nd ed.*, Springer, 2006.

11 - Perturbed Hamiltonian

Moreover, if the stepsize h is not small enough,

sometimes the perturbed Hamiltonian could not well approximate the exact one.

As an example, consider the problem defined by the Hamiltonian:

$$H(q,p) = p^2 + (\beta q)^2 + \alpha(q+p)^{2n}.$$

The corresponding dynamical system has exactly one (marginally stable) equilibrium at the origin.

12 - An example

Let us fix the following parameters [8]:

$$\beta = 10, \qquad \alpha = 1, \qquad n = 4,$$

and suppose we are interested in approximating the level curves of the Hamiltonian passing from the points:

$$(q_0, p_0) = (i, -i), \qquad i = 1, \ldots, 8.$$

This could be done by integrating the trajectories starting at such initial points, for the corresponding Hamiltonian system.

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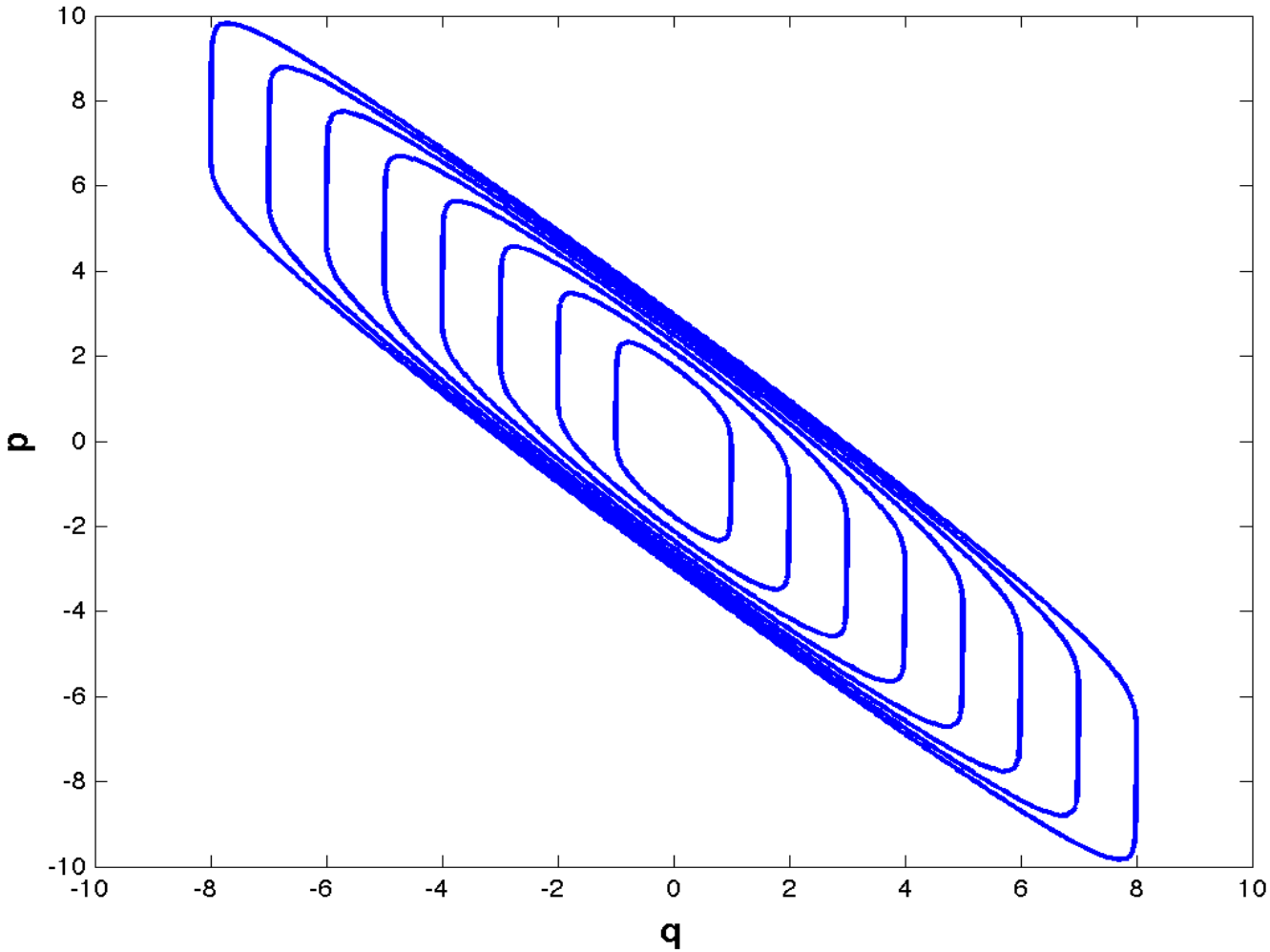
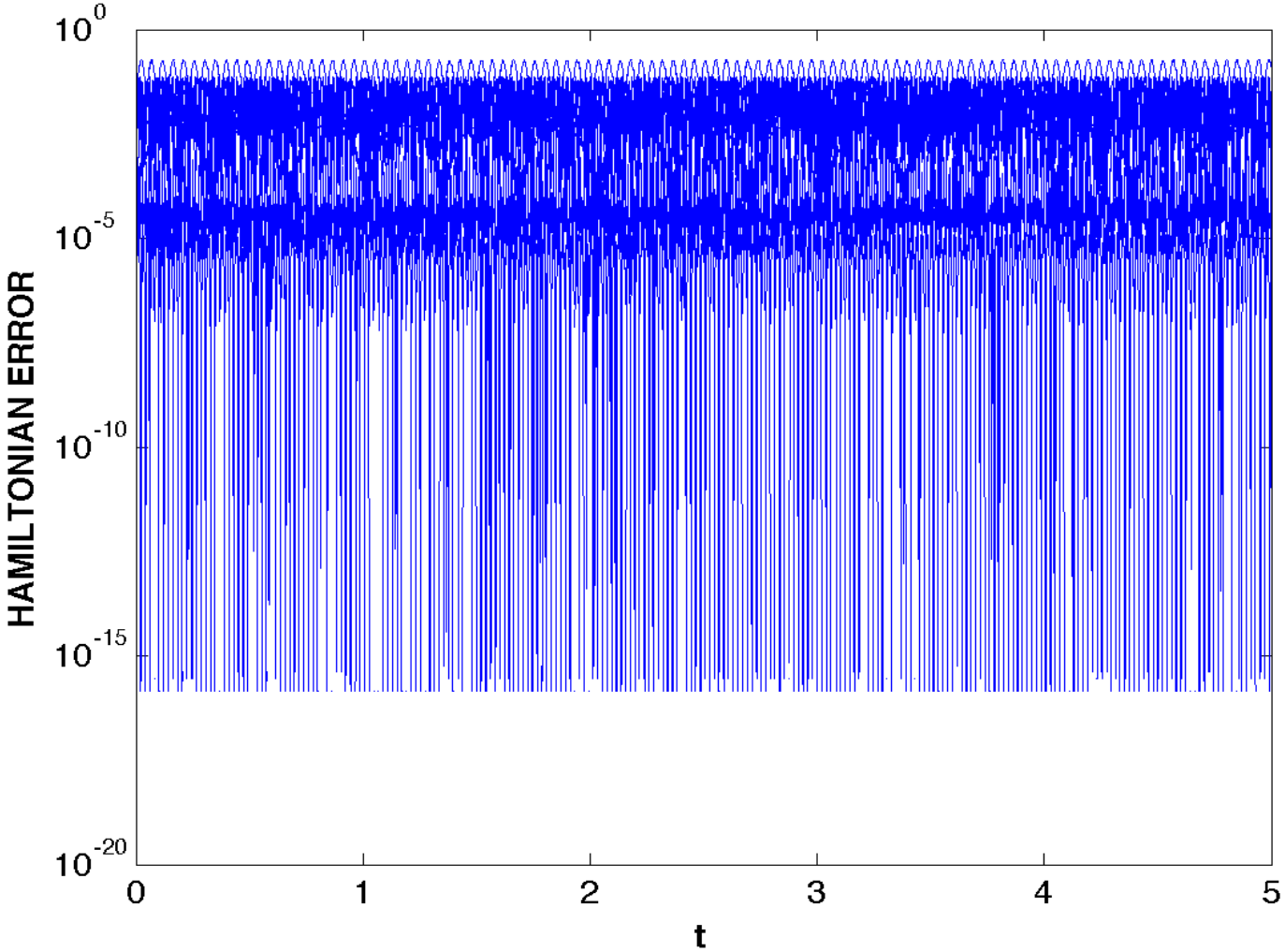
[8] L. B., F. Iavernaro, D. Trigiante. A note on the efficient implementation of Hamiltonian BVMs. *Journal CAM* 236 (2011) 375-383.

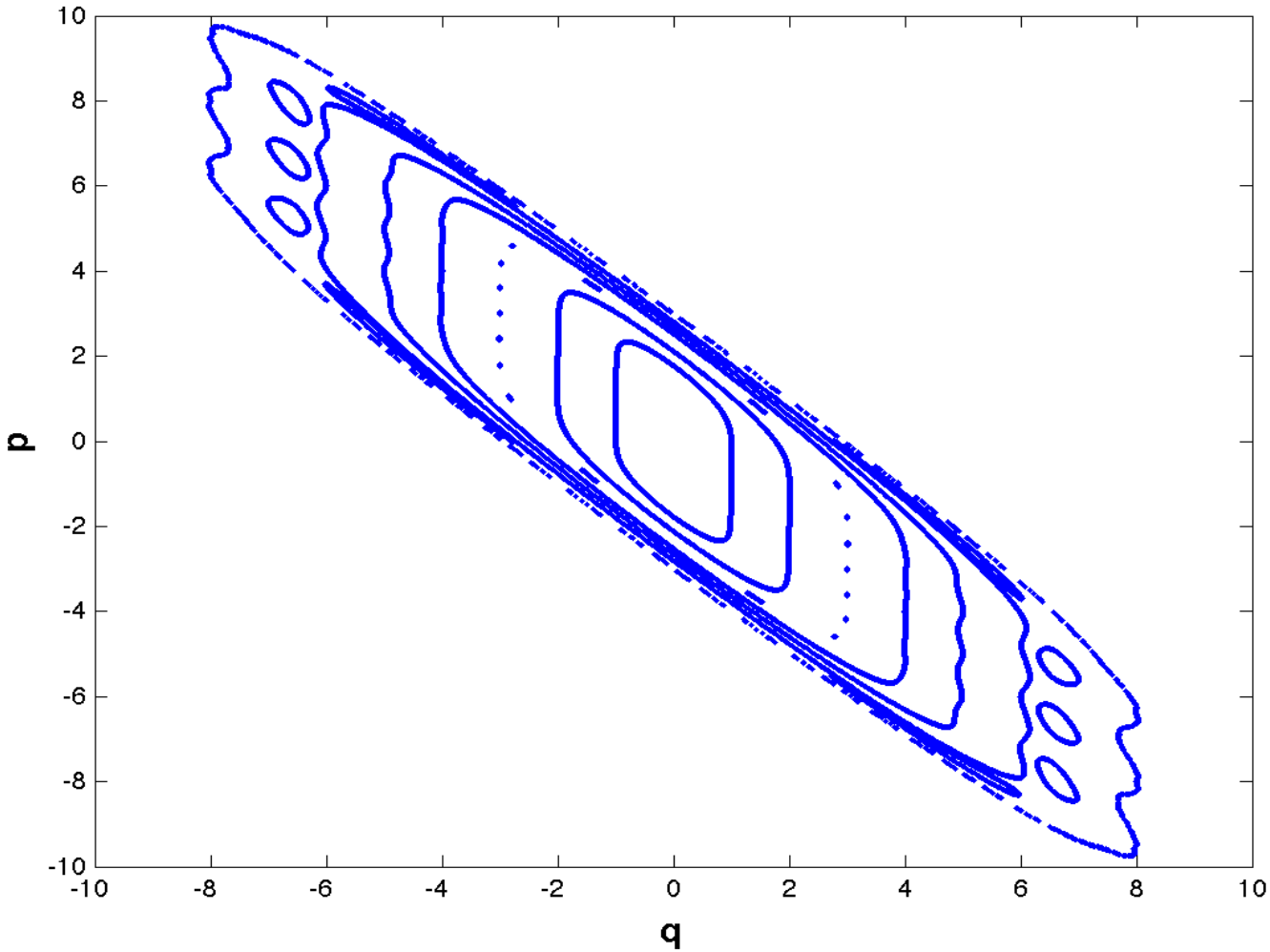
13 - Level curves



14 - 2-stage Gauss method, $h = 10^{-3}$



15 - 2-stage Gauss method, $h = 10^{-3}$



16 - Energy-conserving methods

A way to get rid of this problem is then that of directly looking for energy-conserving methods, able to exactly satisfy the conservation property of the Hamiltonian along the numerical trajectory.

The very first attempts to face this problem were based on projection techniques coupled with standard non-conservative numerical methods.

However, it is well-known that this approach suffers from many drawbacks, in that this is usually not enough to correctly reproduce the long-term dynamics, as is shown, e.g., in [9]

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[9] E. Hairer, C. Lubich, G. Wanner, *Geometric Numerical Integration, 2nd ed.*, Springer, 2006.

17 - Discrete gradient methods

A completely new approach is represented by discrete gradient methods.

They are based upon the definition of a discrete counterpart of the gradient operator, so that energy conservation of the numerical solution is guaranteed at each step and for any choice of the integration step-size [10,11].

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[10] O. Gonzales. Time integration and discrete Hamiltonian systems. *J. Nonlinear Sci.* 6 (1996) 449-467.

[11] R.I. Mc Lachlan, G.R.W. Quispel, N. Robidoux. Geometric integration using discrete gradient. *Phil. Trans. R. Soc. Lond. A* 357 (1999) 1021-1045.

18 - Time finite element methods

A different approach is based on the concept of time finite element methods [12], where one finds local Galerkin approximations on each subinterval of a given mesh of size h for the given ODE-IVPs.

This, in turn, has led to the definition of energy-conserving Runge–Kutta methods [13,14], when replacing the involved integrals with suitable quadrature formulae.

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[12] B.L. Hulme. One-Step Piecewise Polynomial Galerkin Methods for Initial Value Problems. *Mathematics of Computation* 26 (1972) 415-426.

[13] P. Betsch, P. Steinmann. Inherently Energy Conserving Time Finite Elements for Classical Mechanics. *Journal of Computational Physics* 160 (2000) 88-116.

[14] Q. Tang, C.-m. Chen. Continuous finite element methods for Hamiltonian systems. *Applied Mathematics and Mechanics*, 28 (2007) 1071-1080.

19 - Discrete line integral methods

A partially related approach is given by discrete line integral methods [15,16,17].

In such a case, the key idea is to exploit the relation between the method itself and the discrete line integral, i.e., the discrete counterpart of the the line integral in conservative vector fields.

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[15] F. Iavernaro, B. Pace. *s*-Stage Trapezoidal Methods for the Conservation of Hamiltonian Functions of Polynomial Type. *AIP Conf. Proc.* 936 (2007) 603-606. (ICNAAM 2007)

[16] F. Iavernaro, B. Pace. Conservative Block-Boundary Value Methods for the Solution of Polynomial Hamiltonian Systems. *AIP Conf. Proc.* 1048 (2008) 888-891. (ICNAAM 2008)

[17] F. Iavernaro, D. Trigiante. High-order symmetric schemes for the energy conservation of polynomial Hamiltonian problems. *Journal of Numerical Analysis, Industrial and Applied Mathematics* 4,1-2 (2009) 87-101.

20 - Hamiltonian BVMs

The use of discrete line integrals allows, in turn, exact conservation for polynomial Hamiltonians of arbitrarily high-degree.

This resulted in the class of methods later named Hamiltonian Boundary Value Methods (HBVMs), which have been developed in a series of papers (e.g., [18–22]).

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[18] L. B., F. Iavernaro, D. Trigiante. Analisys of Hamiltonian Boundary Value Methods (HBVMs) for the numerical solution of polynomial Hamiltonian dynamical systems, (2009). `arXiv:0909.5659v1`

[19] L. B., F. Iavernaro, D. Trigiante. Hamiltonian BVMs (HBVMs): a family of "drift-free" methods for integrating polynomial Hamiltonian systems. *AIP Conf. Proc.* 1168 (2009) 715-718 (ICNAAM 2009)

[20] L. B., F. Iavernaro, D. Trigiante. Hamiltonian Boundary Value Methods (Energy Preserving Discrete Line Methods). *JNAIAM* 5,1-2 (2010) 17-37.

[21] L. B., F. Iavernaro, D. Trigiante. A note on the efficient implementation of Hamiltonian BVMs. *Journal CAM* 236 (2011) 375-383.

[22] L. B., F. Iavernaro, D. Trigiante. A simple framework for the derivation and analysis of effective one-step methods for ODEs. *Appl. Math. Comput.* 218 (2012) 8475-8485.

21 - Averaged Vector Field method

Another approach, strictly related to the latter one, is given by the Averaged Vector Field method [23,24] and its generalizations [25], which have been mainly analysed in the framework of B-series [26] (i.e., methods admitting a Taylor expansion with respect to the step-size).

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[23] G.R.W. Quispel, D.I. Mc Laren. A new class of energypreserving numerical integration methods. *J. Phys. A: Math. Theor.* 41 (2008) 045206 (7pp).

[24] E. Celledoni, R.I. McLachlan, D. Mc Laren, B. Owren, G.R.W. Quispel, W.M. Wright. Energy preserving RungeKutta methods. *M2AN* 43 (2009) 645-649.

[25] E. Hairer. Energy preserving variant of collocation methods. *JNAIAM* 5,1-2 (2010) 73-84.

[26] E. Hairer, C.J. Zbinden. On conjugate symplecticity of B-series integrators. *IMA J. Numer. Anal.* (2012) 1-23.

22 - HBVMs

The basic idea HBVMs rely on is very simple. Indeed, one has that energy conservation follows as well from the vanishing of the line integral

$$H(y(t)) - H(y_0) = \int_0^t \nabla H(y(s))^T y'(s) \mathrm{d}s = 0,$$

which is due to the fact that

$$y'(s) = J\nabla H(y(s)) \qquad \textit{and} \qquad J^T = -J.$$

23 - A different path

However, one can derive conservation at $t = h$ along any suitable path $\sigma(\cdot)$ joining

$$y_0 = \sigma(0) \qquad \text{to} \qquad y_1 \equiv \sigma(h),$$

such that

$$\begin{aligned} H(y_1) - H(y_0) \;&\equiv\; H(\sigma(h)) - H(\sigma(0)) \\ &= \int_0^h \nabla H(\sigma(s))^T \sigma'(s) \mathrm{d}s \\ &= h \int_0^1 \nabla H(\sigma(\tau h))^T \sigma'(\tau h) \mathrm{d}\tau \;=\; 0. \end{aligned}$$

24 - Polynomial path

We choose σ to be a polynomial of degree s, and expand its derivative along a suitable polynomial basis $\{P_j\}_{j\geq 0}$:

$$\sigma'(ch) = \sum_{j=0}^{s-1} \gamma_j P_j(c), \qquad c \in [0,1].$$

By imposing the condition $\sigma(0) = y_0$, one obtains, formally,

$$\sigma(ch) = y_0 + h \sum_{j=0}^{s-1} \gamma_j \int_0^c P_j(\tau) \mathrm{d}\tau, \qquad c \in [0,1].$$

25 - Orthonormal basis

In particular, we choose, as polynomial basis, the Legendre polynomials, which are shifted on the interval $[0, 1]$, and scaled such that they are orthonormal:

$$\int_0^1 P_i(c) P_j(c) \mathrm{d}c = \delta_{ij}, \qquad \forall i, j \geq 0.$$

26 - Energy conservation

By imposing the vanishing of the line integral to obtain energy conservation, one has

$$\begin{aligned} 0 &= \int_0^1 \nabla H(\sigma(\tau h))^T \overbrace{\sum_{j=0}^{s-1} \gamma_j P_j(\tau)}^{=\sigma'(\tau h)} \mathrm{d}\tau \\ &= \sum_{j=0}^{s-1} \left(\int_0^1 \nabla H(\sigma(\tau h)) P_j(\tau) \mathrm{d}\tau \right)^T \gamma_j. \end{aligned}$$

In view of the skew-symmetry of matrix J, this holds true by choosing the (vector) coefficients γ_j as

$$\gamma_j = J \int_0^1 \nabla H(\sigma(\tau h)) P_j(\tau) \mathrm{d}\tau, \quad j = 0, \ldots, s-1.$$

27 - Discrete problem

With this choice, the nonlinear system defining the unknown coefficients γ_j becomes, by setting $f(\cdot) = J\nabla H(\cdot)$,

$$\gamma_j = \int_0^1 P_j(\tau) \overbrace{f\left(y_0 + h\sum_{i=0}^{s-1}\gamma_i \int_0^\tau P_i(c)\mathrm{d}c\right)}^{=f(\sigma(\tau h))} \mathrm{d}\tau,$$
$$j = 0, \ldots, s-1.$$

By considering that $P_0(\tau) \equiv 1$, the new approximation is then given by

$$y_1 \equiv \sigma(h) = y_0 + h\gamma_0.$$

We stress, however, that the previous formulae do not represent an operative method unless the integrals are approximated by means of a suitable quadrature formula.

28 - HBVM(k,s)

For this purpose, let us consider the interpolation quadrature formula defined at the abscissae

$$0 \leq c_1 < \cdots < c_k \leq 1,$$

and the corresponding weights $\{b_i\}$. The final shape of a HBVM method, denoted by HBVM(k,s), is then given by

$$\begin{aligned} \gamma_j &= \sum_{\ell=1}^{k} b_\ell P_j(c_\ell) f\left(y_0 + h \sum_{i=0}^{s-1} \gamma_i \int_0^{c_\ell} P_j(c)\mathrm{d}c \right), \\ & \qquad j = 0, \ldots, s-1, \end{aligned}$$

which is a system of s nonlinear vector algebraic equations in the unknowns $\{\gamma_j\}$, for any value of k.

29 - Runge-Kutta formulation

Substituting the obtained expression of γ_j into

$$\sigma(ch) = y_0 + h\sum_{j=0}^{s-1}\gamma_j\int_0^c P_j(\tau)\mathrm{d}\tau, \qquad c \in [0,1],$$

and setting

$$Y_i = \sigma(c_i h), \qquad i = 1,\ldots,k,$$

one then obtains:

$$Y_i = y_0 + h\sum_{j=0}^{s-1}\int_0^{c_i} P_j(s)\mathrm{d}s\sum_{\ell=1}^{k} b_\ell P_j(c_\ell) f(Y_\ell), \quad i = 1,\ldots,k,$$

with the new approximation given by

$$y_1 = y_0 + h\sum_{i=1}^{s} b_i f(Y_i).$$

30 - Runge-Kutta form of HBVMs

Evidently, the previous equations represent the following k-stage Runge-Kutta method,

$$\begin{array}{c|c} c_1 & \\ \vdots & A \equiv \left(b_j \sum_{\ell=0}^{s-1} P_\ell(c_j) \int_0^{c_i} P_\ell(x)\mathrm{d}x \right)_{i,j=1,\ldots,k} \\ c_k & \\ \hline & b_1 \quad \ldots \quad b_k \end{array}$$

defining the Runge-Kutta shape of a HBVM(k, s) method.

31 - Quadrature

Assume to place the nodes at the k Gauss-Legendre points in $[0, 1]$. Then, for all $k \geq s$, HBVM(k, s):

- has order $2s$,
- the quadrature is exact for all polynomial Hamiltonians of degree no larger than

$$\nu \leq \frac{2k}{s},$$

- for general (suitably regular) Hamiltonians, the energy error is

$$O(h^{2k+1}),$$

thus implying a practical conservation, provided that k is large enough, also in the non-polynomial case.

32 - Matrix form

We can easily express the Butcher matrix of an HBVM(k,s) by introducing the following matrices:

$$\mathcal{P}_s = \begin{pmatrix} P_0(c_1) & \dots & P_{s-1}(c_1) \\ \vdots & & \vdots \\ P_0(c_k) & \dots & P_{s-1}(c_k) \end{pmatrix},$$

$$\mathcal{I}_s = \begin{pmatrix} \int_0^{c_1} P_0(x)\mathrm{d}x & \dots & \int_0^{c_1} P_{s-1}(x)\mathrm{d}x \\ \vdots & & \vdots \\ \int_0^{c_k} P_0(x)\mathrm{d}x & \dots & \int_0^{c_k} P_{s-1}(x)\mathrm{d}x \end{pmatrix} \in \mathbb{R}^{k\times s}$$

33 - Structure matrix

They are related as follows,

$$\mathcal{I}_s = \mathcal{P}_{s+1}\hat{X}_s,$$

via the structure matrix:

$$\hat{X}_s = \left(\begin{array}{cccc} \frac{1}{2} & -\xi_1 & & \\ \xi_1 & 0 & \ddots & \\ & \ddots & \ddots & -\xi_{s-1} \\ & & \xi_{s-1} & 0 \\ \hline & & & \xi_s \end{array}\right) \equiv \left(\begin{array}{c} X_s \\ \hline 0 \ \ldots \ 0 \ \xi_s \end{array}\right) \in \mathbb{R}^{s+1 \times s},$$

with $\xi_i = (2\sqrt{4i^2 - 1})^{-1}, \quad i = 1, \ldots, s.$

34 - Matrix form

By also introducing the diagonal matrix with the quadrature weights,

$$\Omega = \begin{pmatrix} b_1 & & \\ & \ddots & \\ & & b_k \end{pmatrix} \in \mathbb{R}^{k \times k},$$

we finally obtain

$$A = \mathcal{I}_s \mathcal{P}_s^T \Omega \equiv \underbrace{\mathcal{P}_{s+1} \hat{X}_s}_{= \mathcal{I}_s} \mathcal{P}_s^T \Omega \in \mathbb{R}^{k \times k},$$

whose rank is s.

35 - Generalized W-transform

In general, $k \geq s$. In the case $k = s$, one obtains due to the fact that $P_s(c_i) = 0$, $i = 1, \ldots, s$,

$$\mathcal{P}_{s+1} = \begin{pmatrix} \mathcal{P}_s & 0 \end{pmatrix}, \qquad \mathcal{P}_s^{-1} = \mathcal{P}_s^T \Omega,$$

so that we obtain the s-stage Gauss method,

$$A = \mathcal{P}_s X_s \mathcal{P}_s^{-1}.$$

In this sense, for $k \geq s$,

$$A = \mathcal{P}_{s+1} \hat{X}_s \mathcal{P}_s^T \Omega$$

can be regarded as a generalized W-transfrom [27].

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[27] E. Hairer, G. Wanner. *Solving Differential Equations II*. Springer, 1991.

36 - Isospectral property of HBVMs

From the previous result, it follows that, for all $k \geq s$, HBVM(k,s) share the same spectrum.

Indeed, the matrix

$$A = \mathcal{P}_{s+1} \hat{X}_s \mathcal{P}_s^T \Omega \in \mathbb{R}^{k \times k}$$

has constant rank s, so that it has a $(k-s)$-fold 0 eigenvalue. The remaining ones can be easily seen to coincide with the s eigenvalues of X_s (i.e., those of the Butcher matrix of the s-stage Gauss method) [28].

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[28] L.B., F. Iavernaro, D. Trigiante. The Lack of Continuity and the Role of Infinite and Infinitesimal in Numerical Methods for ODEs: the Case of Symplecticity. *Appl. Math. Comput.* 218 (2012) 8053–8063.

37 - Computational issues

The low-rank structure of the Butcher matrix of HBVM(k,s), allows to make their implementation more efficient.
Indeed, by setting Y the block vector of dimension k with the stages of the method, one has to solve

$$Y = 1 \otimes y_0 + h(\mathcal{I}_s \underbrace{\mathcal{P}_s^T \Omega}_{=\gamma}) \otimes I\, f(Y),$$

where $f(Y) \equiv J\nabla H(Y)$ is a block vector. By setting

$$\gamma = \mathcal{P}_s^T \Omega \otimes I\, f(Y)$$

the block vector of dimension s with the coefficients of the polynomial σ, one has

$$Y = 1 \otimes y_0 + h\mathcal{I}_s \otimes I\gamma,$$

and, then,

$$\gamma = \mathcal{P}_s^T \Omega \otimes I\, f\left(1 \otimes y_0 + h\mathcal{I}_s \otimes I\gamma\right).$$

38 - Some examples

Let us consider again the problems defined by the Hamiltonian:

$$H(q,p) = p^2 + (\beta q)^2 + \alpha(q+p)^{2n},$$

with parameters

$$\beta = 10, \qquad \alpha = 1, \qquad n = 4,$$

and initial points:

$$(q_0, p_0) = (i, -i), \qquad i = 1, \ldots, 8.$$

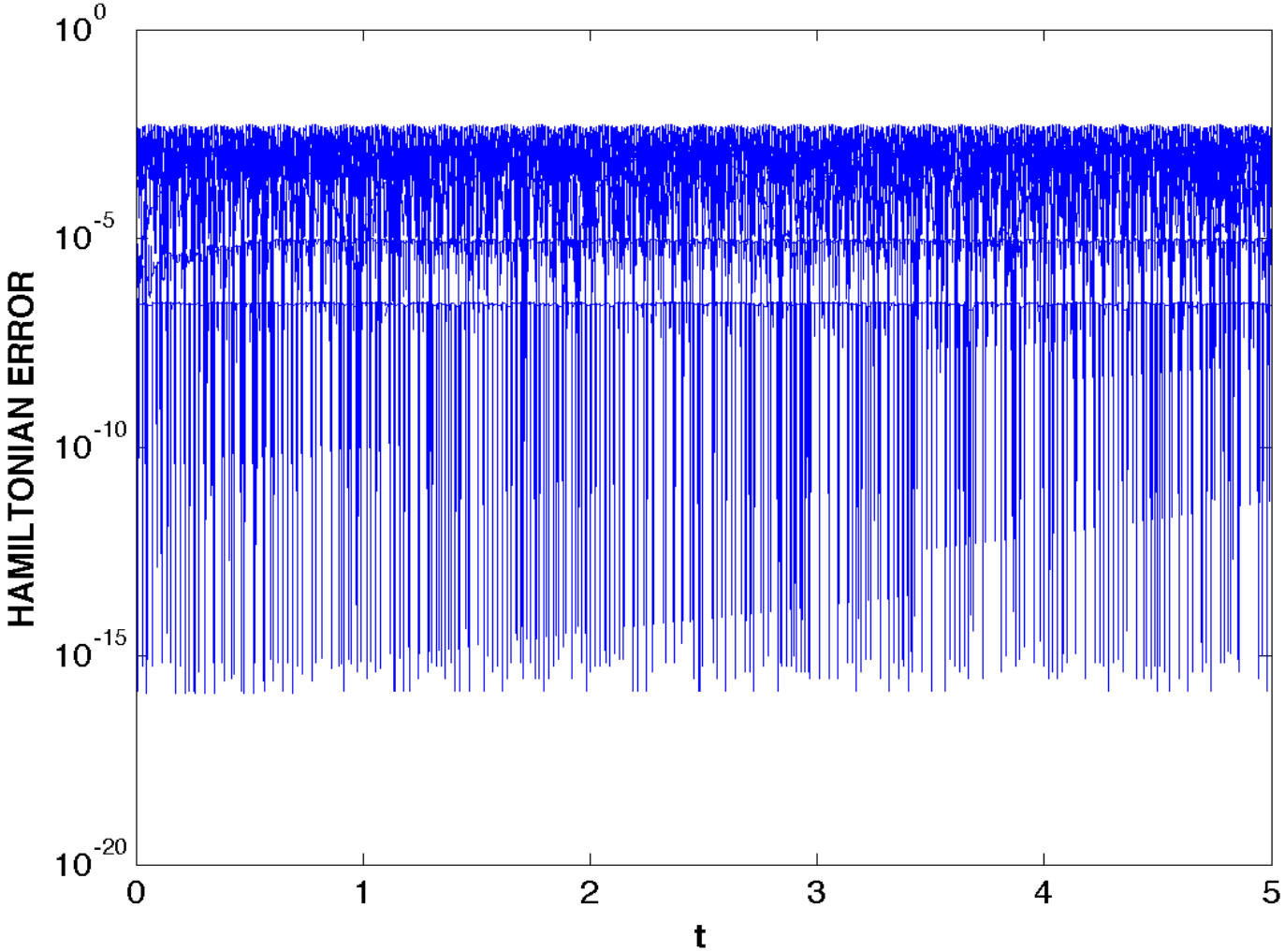
We use the HBVM(k,s) method with $s = 2$ and $k \geq s$, so that the method has order 4, with the same stepsize $h = 10^{-3}$ as before.

39 - fourth-order HBVM(k,2) method

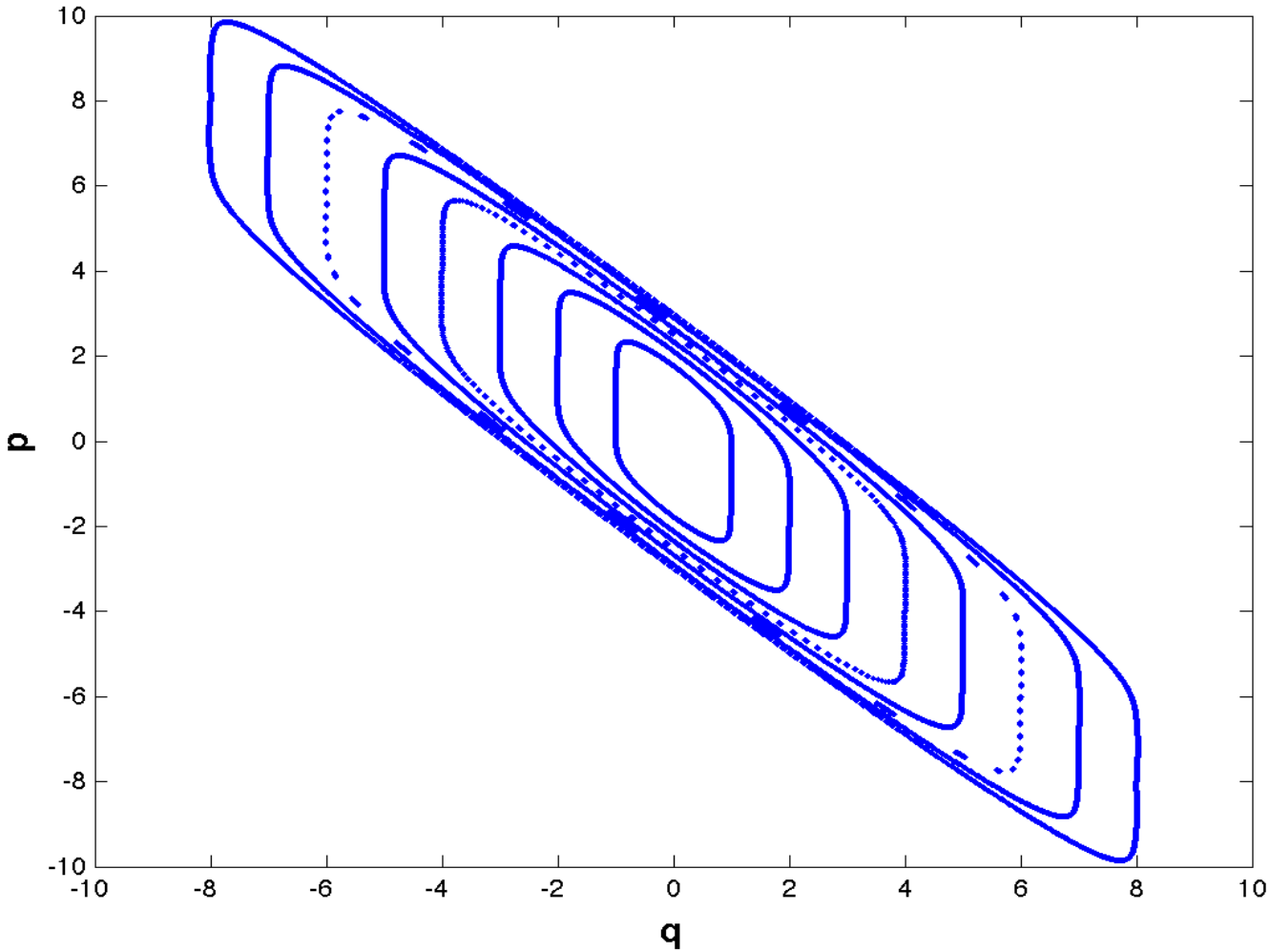
By placing the k abscissae $c_1, \ldots, c_k$ for the quadrature at the Gauss-Legendre points in [0,1], we have that the error in the Hamiltonian is:

- $O(h^{2k+1})$ for $k = 2, 3, \ldots, 7$;
- in particular, for $k = 2$ we recover the 2-stage Gauss method;
- 0, for $k \geq 8$, due to the fact that the Hamiltonian is a polynomial of degree 8.

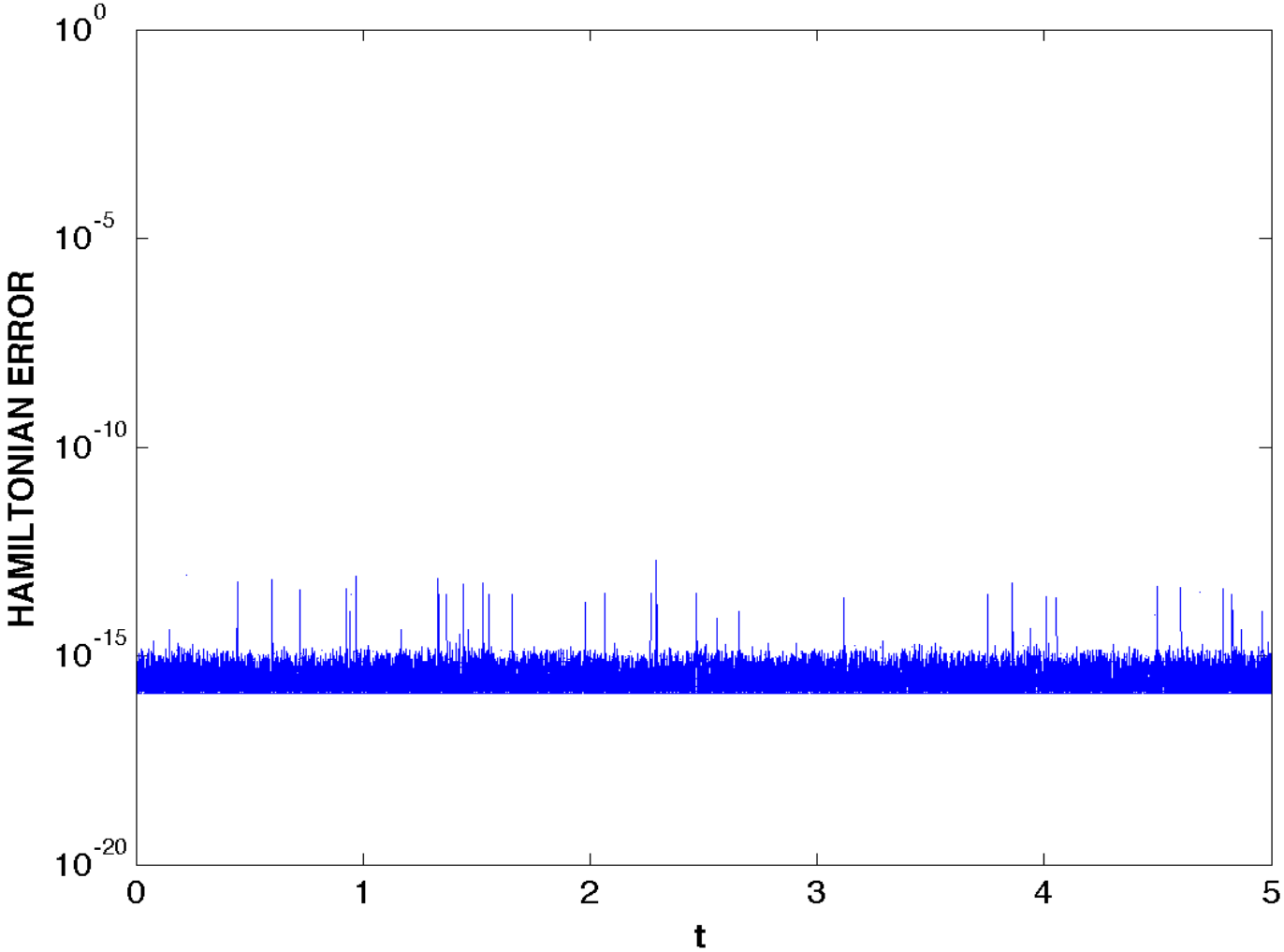
40 - HBVM(3,2) method, $h = 10^{-3}$



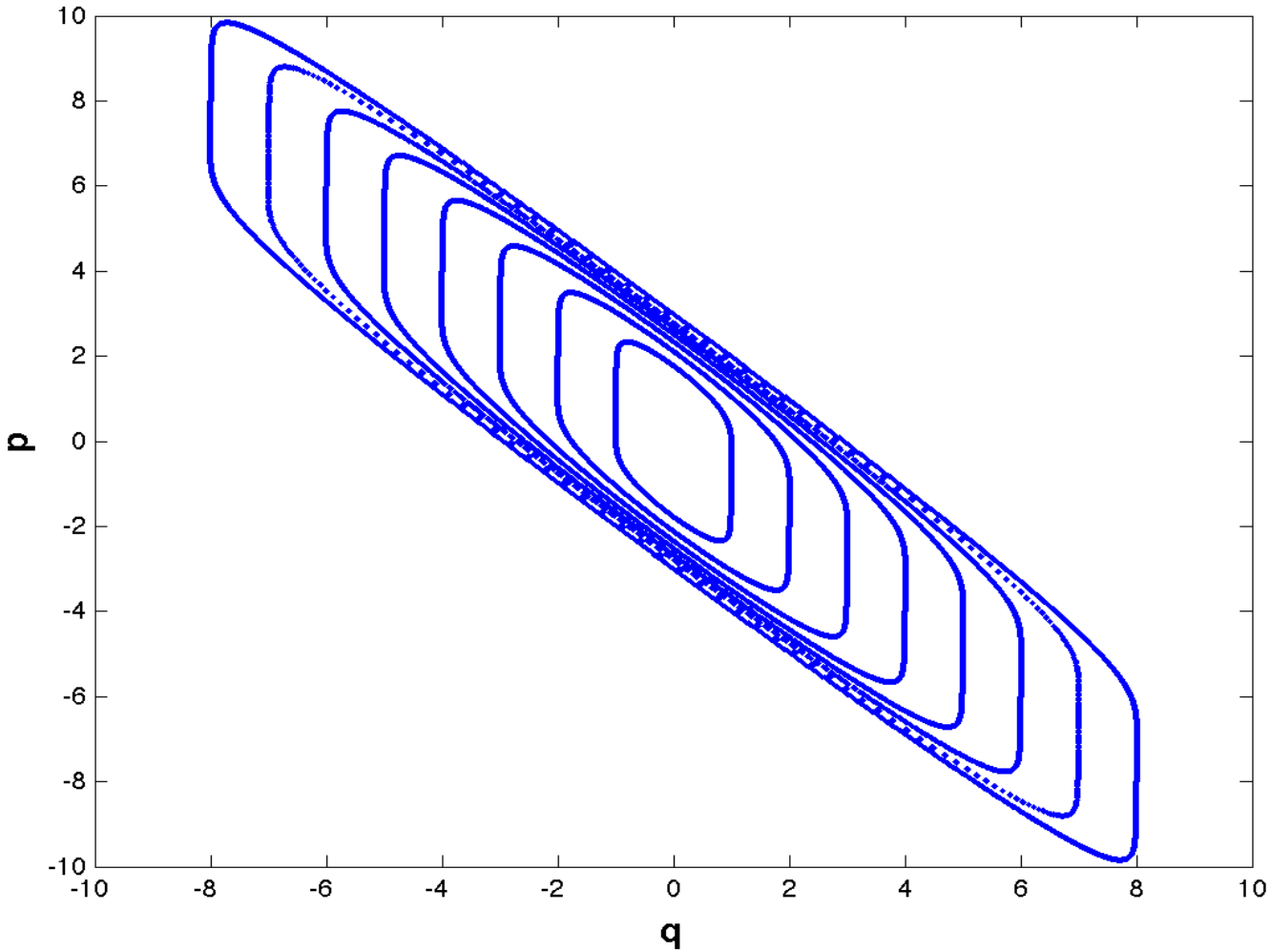
41 - HBVM(3,2) method, $h = 10^{-3}$



42 - HBVM(8,2) method, $h = 10^{-3}$



43 - HBVM(8,2) method, $h = 10^{-3}$



44 - Generalizations

It is worth mentioning that the basic idea on which HBVMs rely, can be extended to cope with any conservative problems.

Indeed, let us suppose that a general ODE-IVPs,

$$y' = f(y), \qquad y(0) = y_0,$$

has ν (independent) smooth invariants:

$$L(y(t)) = L(y_0) \in \mathbb{R}^\nu, \qquad t \geq 0.$$

45 - Modified polynomial method

The basic idea is now that of modifying the form of the polynomial $\sigma(\cdot)$ as follows:

$$\sigma'(ch) = \underbrace{\sum_{j=0}^{s-1} \gamma_j P_j(c)}_{original} + \overbrace{\phi_0 \alpha}^{additional}, \qquad c \in [0,1],$$

with

$$\alpha \in \mathbb{R}^{\nu},$$

and, in general,

$$\phi_j = \int_0^1 P_j(\tau) J_L^T(\sigma(\tau h)) \mathrm{d}\tau, \qquad j \geq 0,$$

being $J_L(\cdot)$ the Jacobian matrix of $L(\cdot)$.

46 - Conservation through the line integral

By imposing, as usual, the conservation through a line integral, one then obtains:

$$\begin{aligned} 0 &= L(\sigma(h)) - L(\sigma(0)) = h \int_0^1 J_L(\sigma(\tau h))\sigma'(\tau h))\mathrm{d}\tau \\ &= h \left(\sum_{j=0}^{s-1} \phi_j^T \gamma_j \; + \; \phi_0^T \phi_0 \alpha \right). \end{aligned}$$

Which is satisfied provided that

$$\underbrace{\left(\phi_0^T \phi_0\right)}_{\text{spd ``matrix''}} \alpha = -\sum_{j=0}^{s-1} \phi_j^T \gamma_j.$$

47 - Line Integral Methods (LIMs)

By suitably discretizing the involved integrals, one obtains the class of methods, which has been named

Line Integral Methods (LIMs)

$$\text{LIM}\Big(\underbrace{r}_{\phi_j \text{ quadrature}}, \overbrace{k}^{\gamma_j \text{ quadrature}}, \underbrace{s}_{\text{degree of } \sigma}\Big)$$

In particular:

- LIM(0,k,s) coincide with HBVM(k,s);
- LIM(0,s,s) coincide with s-stage Gauss methods.

48 - Line Integral Methods (LIMs)

Fully conservative variants of both:

- HBVM(k,s) methods, i.e., LIM(k,k,s), and
- s-stage Gauss-Legendre methods, i.e., LIM(k,s,s),

are reported in [29].

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[29] L.Brugnano, F.Iavernaro. Line Integral Methods which preserve all invariants of conservative problems. *Journal CAM* 236 (2012) 3905–3919.

Also presented at ICNAAM 2011.

49 - Symplectic low-rank Runge-Kutta methods

A noticeable extension of symplectic Gauss-Legendre methods has been recently devised in [30], starting from the Runge-Kutta formulation of HBVMs, which have been called Symplectic low-rank Runge-Kutta methods.

They can be quite straightforwardly obtained from the matrix form of HBVM(k,s).

$$\begin{array}{c|c} c_1 & \\ \vdots & A \equiv \mathcal{P}_{s+1}\hat{X}_s\mathcal{P}_s^T\Omega \\ c_k & \\ \hline & b_1 \quad \dots \quad b_k \end{array}$$

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[30] K. Burrage, P.M. Burrage. Low rank Runge-Kutta methods, symplecticity and stochastic Hamiltonian problems with additive noise. *Journal CAM* 236 (2012) 3920–3930.

50 - Involved matrices

$$\mathcal{P}_s = \begin{pmatrix} P_0(c_1) & \dots & P_{s-1}(c_1) \\ \vdots & & \vdots \\ P_0(c_k) & \dots & P_{s-1}(c_k) \end{pmatrix} \in \mathbb{R}^{k \times s},$$

$$\hat{X}_s = \left(\begin{array}{cccc} \frac{1}{2} & -\xi_1 & & \\ \xi_1 & 0 & \ddots & \\ & \ddots & \ddots & -\xi_{s-1} \\ & & \xi_{s-1} & 0 \\ \hline & & & \xi_s \end{array}\right) \equiv \left(\begin{array}{c} X_s \\ \hline 0 \dots 0 \ \xi_s \end{array}\right) \in \mathbb{R}^{s+1 \times s},$$

$$\Omega = \operatorname{diag}(b_1, \dots, b_k).$$

51 - Symplecticity criterion for Runge-Kutta methods

By using the criterion for symplecticity stated in [31] on the HBVM(k,s) method, one has, by setting $b = \Omega 1$:

$$\Omega A + A^T \Omega - bb^T = \xi_s \left(v_s v_{s-1}^T + v_{s-1} v_s^T \right),$$

with

$$v_r = \left(\begin{array}{ccc} b_1 P_r(c_1) & \dots & b_k P_r(c_k) \end{array} \right)^T, \qquad r = s-1, s,$$

so that the method is not symplectic.

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[31] J.M. Sanz-Serna. Runge-Kutta schemes for Hamiltonian systems. *BIT* 28 (1988) 877-883.

52 - SLIRK(k,s)

However, by setting

$$\xi_s = 0$$

one obtains that the following method, denoted by SLIRK(k,s), is trivially symplectic:

$$\begin{array}{c|c} c_1 & \\ \vdots & A \equiv \mathcal{P}_s X_s \mathcal{P}_s^T \Omega \\ c_k & \\ \hline & b_1 \quad \ldots \quad b_k \end{array}$$

The rank of A is obviously s, for all $k \geq s$.

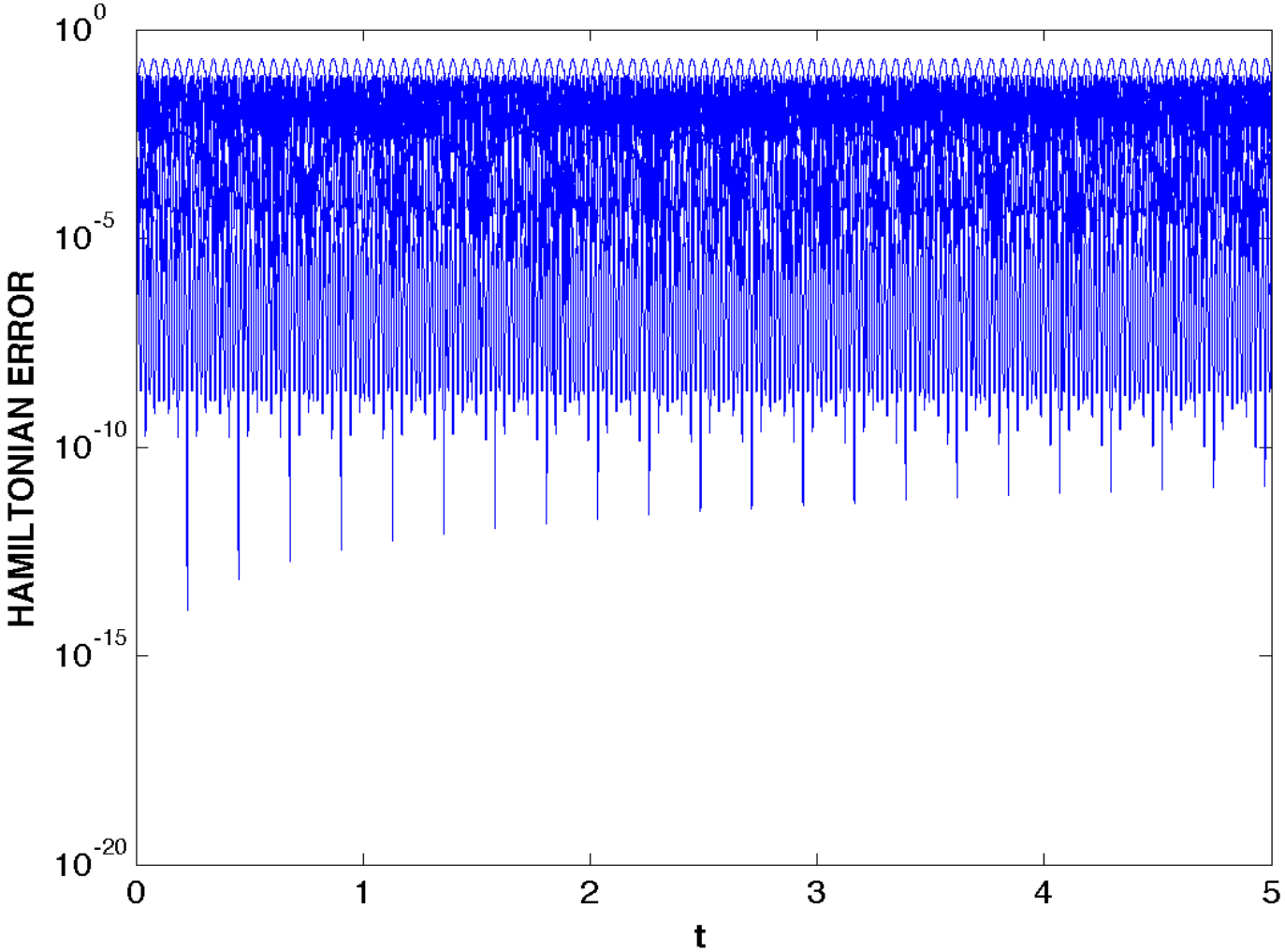
53 - Energy error

SLIRK(k,s) inherit many properties of the underlying s-stage Gauss method, which is obtained when $k = s$ and the abscissae are placed at the Gauss-Legendre nodes in [0,1]:

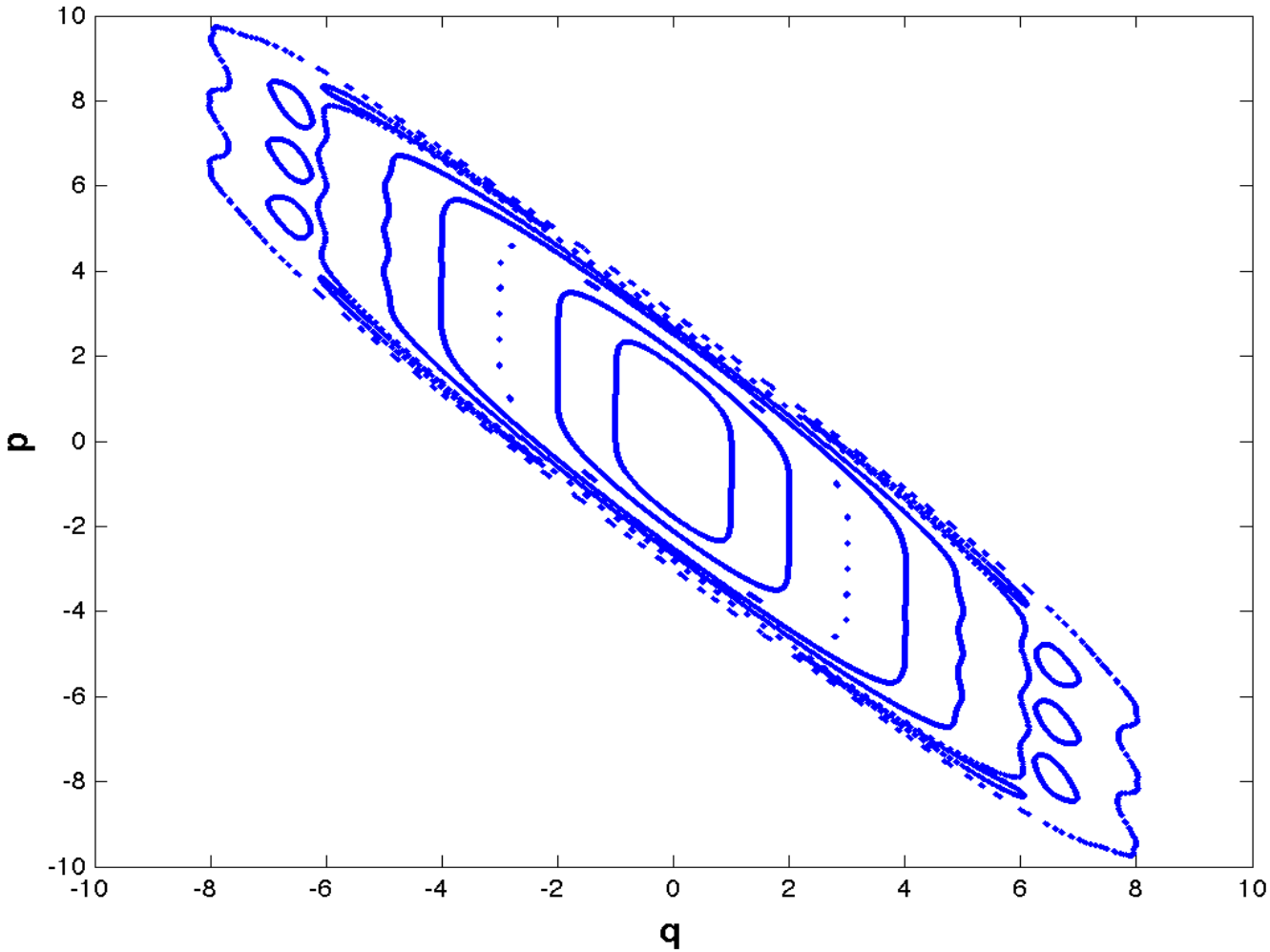
- it is symmetric and symplectic;
- it has order 2s;
- the Hamiltonian error is of the same order.

It cannot improve over such method.

54 - SLIRK(8,2), $h = 10^{-3}$



55 - SLIRK(8,2), $h = 10^{-3}$



56 - Nevertheless . . .

Let consider a separable Hamiltonian problem with additive noise,

$$\begin{aligned} \mathrm{d}q &= p\mathrm{d}t, \qquad q(0) = q_0, \\ \mathrm{d}p &= -V'(q)\mathrm{d}t + \sigma \mathrm{d}W, \qquad p(0) = p_0, \end{aligned}$$

with the Hamiltonian

$$H(q,p) = \frac{1}{2}p^2 + V(q),$$

and $W(t)$ a Wiener process satisfying

$$\langle W(t)W(s)\rangle = \min(t,s).$$

57 - SLIRK(k,s) for stochastic Hamiltonian problems

The solution of the above problem is formally given by

$$\begin{aligned} q(t) &= q_0 + \int_0^t p(\tau)\mathrm{d}\tau, \\ p(t) &= p_0 - \int_0^t V'(q(\tau))\mathrm{d}\tau + \overbrace{\int_0^t \sigma \mathrm{d}W(\tau)}^{\textit{stochastic integral}} . \end{aligned}$$

In such a case, the use of a higher value of k allows a better approximation of the involved stochastic integral, and better statistical results are reported in [32], w.r.t. the underlying s-stage Gauss method.

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[32] K. Burrage, P.M. Burrage. Low rank Runge-Kutta methods, symplecticity and stochastic Hamiltonian problems with additive noise. *Journal CAM* 236 (2012) 3920–3930.

58 - Symplecticity and Energy conservation

Is it possible, for a numerical method, to have both the symplecticness of the map and the energy-conservation property?

Attempts to incorporate both symplecticity and energy conservation into the numerical method will clash with

two non-existence results.

The first [33] refers to non-integrable systems, that is systems that do not admit other independent first integrals different from the Hamiltonian function itself:

If [the method] is symplectic, and conserved H exactly, then it is the time advance map for the exact Hamiltonian system up to a reparametrization of time.

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[33] Z. Ge, J.E. Marsden. Lie-Poisson Hamilton-Jacobi theory and Lie-Poisson integrators. *Phys. Lett. A* 133 (1988) 134–139.

59 - Further non-existence result

The second negative result [34] refers to B-series symplectic methods applied to general (not necessarily non-integrable) Hamiltonian systems:

The only symplectic method (as B-series) that conserves the Hamiltonian for arbitrary $H(y)$ is the exact flow of the differential equation.

---

[34] P. Chartier, E. Faou, A. Murua. An algebraic approach to invariant preserving integrators: the case of quadratic and Hamiltonian invariants. *Numer. Math.* 103, no. 4 (2006) 575–590.

60 - Nevertheless...

The impossibility for a constant time stepping algorithm to be at the same time symplectic and energy-conserving has led to research into methods which could inherit both features in a weaker sense.

This delicate aspect has been thoroughly faced in [35] where the authors prove the existence of symplectic-energy-momentum preserving integrators by using time-adaptive steps.

Here time-step adaption is used to impose energy conservation (see also [36]).

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[35] C. Kane, J.E. Marsden, M. Ortiz. Symplectic-energy-momentum preserving variational integrators. *Jour. Math. Phys.* 40, no. 7 (1999) 3353–3371.

[36] J.E. Marsden, J.M. Wendlandt. Mechanical Systems with Symmetry, Variational Principles, and Integration Algorithms, in *Current and Future Directions in Applied Mathematics*, M. Alber, B. Hu, J. Rosenthal, Eds. Birkhauser, 1997, pp. 219–261.

61 - EQUIP methods

By following a different route, in [37,38,39] a new class of methods, named

Energy and QUadratic Invariants Preserving (EQUIP) methods,

has been defined. Their straightforward formulation can be easily sketched by using the framework of matrices.

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[37] L. Brugnano, F. Iavernaro, D. Trigiante. Energy and quadratic invariants preserving integrators of Gaussian type. *AIP Conf. Proc.* 1281 (2010) 227–230. (ICNAAM 2010)

[38] L. Brugnano, F. Iavernaro, D. Trigiante. Numerical comparisons among some methods for Hamiltonian problems . *AIP Conf. Proc.* 1281 (2010) 214–218. (ICNAAM 2010)

[39] L. Brugnano, F. Iavernaro, D. Trigiante. Energy and quadratic invariants preserving integrators based upon Gauss collocation formulae. *SIAM J. Numer. Anal.* (to appear)

62 - Matrix framework

Let consider the W-transform of the Butcher matrix of the s-stage Gauss method:

$$A = \mathcal{P}_s X_s \mathcal{P}_s^T \Omega,$$

which satisfies the conservation property for quadratic invariants, i.e.,

$$\Omega A + A^T \Omega - bb^T = \Omega \mathcal{P}_s (X_s + X_s^T) \mathcal{P}_s^T \Omega - bb^T = 0,$$

due to the fact that

$$X_s + X_s^T = e_1 e_1^T$$

and

$$\Omega(\mathcal{P}_s e_1) = \Omega 1 = b.$$

63 - EQUIP variant of Gauss methods

The above property continues to hold, provided that we replace matrix X_s by

$$X_s(\alpha) = X_s + \alpha W,$$

with $W^T = -W$, due to the fact that

$$X_s(\alpha) + X_s(\alpha)^T = X_s + X_s^T + \alpha \overbrace{(W + W^T)}^{=0} = X_s + X_s^T.$$

The free parameter α can be chosen in order to get, at each integration step, energy-conservation.

In particular, by setting

$$X_s(\alpha) = \begin{pmatrix} \frac{1}{2} & -\xi_1 & & & & & \\ \xi_1 & 0 & \ddots & & & & \\ & \ddots & \ddots & -(\xi_i+\alpha) & & & \\ & & (\xi_i+\alpha) & \ddots & \ddots & & \\ & & & \ddots & \ddots & -\xi_{s-1} & \\ & & & & \xi_{s-1} & 0 & \end{pmatrix},$$

it can be proved that $\alpha = O(h^{2(s-i)})$, so that the order $2s$ of the original Gauss method is retained by its EQUIP variant [40].

---

[40] L. Brugnano, F. Iavernaro, D. Trigiante. Energy and quadratic invariants preserving integrators based upon Gauss collocation formulae. *SIAM J. Numer. Anal.* (to appear)

65 - EQUIP variant of the 2-stage Gauss method

As an example, for $s = 2$, one obtains,

$$X_2(\alpha) = \begin{pmatrix} \frac{1}{2} & -(\xi_1 + \alpha) \\ (\xi_1 + \alpha) & 0 \end{pmatrix},$$

from which one obtains the fourth-order EQUIP variant:

$$\begin{array}{c|cc} \frac{1}{2} - \frac{\sqrt{3}}{6} & \frac{1}{4} & \frac{1}{4} - \frac{\sqrt{3}}{6} - \alpha \\ \frac{1}{2} + \frac{\sqrt{3}}{6} & \frac{1}{4} + \frac{\sqrt{3}}{6} + \alpha & \frac{1}{4} \\ \hline & \frac{1}{2} & \frac{1}{2} \end{array}$$

When $\alpha = 0$ one retrieves the original 2-stage Gauss method.

66 - EQUIP variants of the 3-stage Gauss method

In such case, we have the following two sixth-order EQUIP variants:

- First variant:

$$X_3(\alpha) = \begin{pmatrix} \frac{1}{2} & -(\xi_1 + \alpha) & 0 \\ (\xi_1 + \alpha) & 0 & -\xi_2 \\ 0 & \xi_2 & 0 \end{pmatrix},$$

  with $\alpha = O(h^4)$;

- Second variant:

$$X_3(\alpha) = \begin{pmatrix} \frac{1}{2} & -\xi_1 & 0 \\ \xi_1 & 0 & -(\xi_2 + \alpha) \\ 0 & (\xi_2 + \alpha) & 0 \end{pmatrix},$$

  with $\alpha = O(h^2)$;

67 - First sixth-order EQUIP variant

$$
\begin{array}{c|cccc}
\frac{1}{2}-\frac{\sqrt{15}}{10} & \frac{5}{36} & \frac{2}{9}-\frac{\sqrt{15}}{15}-4\alpha\frac{\sqrt{5}}{15} & \frac{5}{36}-\frac{\sqrt{15}}{30}-\alpha\frac{\sqrt{5}}{3} \\
\frac{1}{2} & \frac{5}{36}+\frac{\sqrt{15}}{24}+\alpha\frac{\sqrt{5}}{6} & \frac{2}{9} & \frac{5}{36}-\frac{\sqrt{15}}{24}-\alpha\frac{\sqrt{5}}{6} \\
\frac{1}{2}+\frac{\sqrt{15}}{10} & \frac{5}{36}+\frac{\sqrt{15}}{30}+\alpha\frac{\sqrt{5}}{3} & \frac{2}{9}+\frac{\sqrt{15}}{15}+4\alpha\frac{\sqrt{5}}{15} & \frac{5}{36} \\
\hline
 & \frac{5}{18} & \frac{4}{9} & \frac{5}{18}
\end{array}
$$

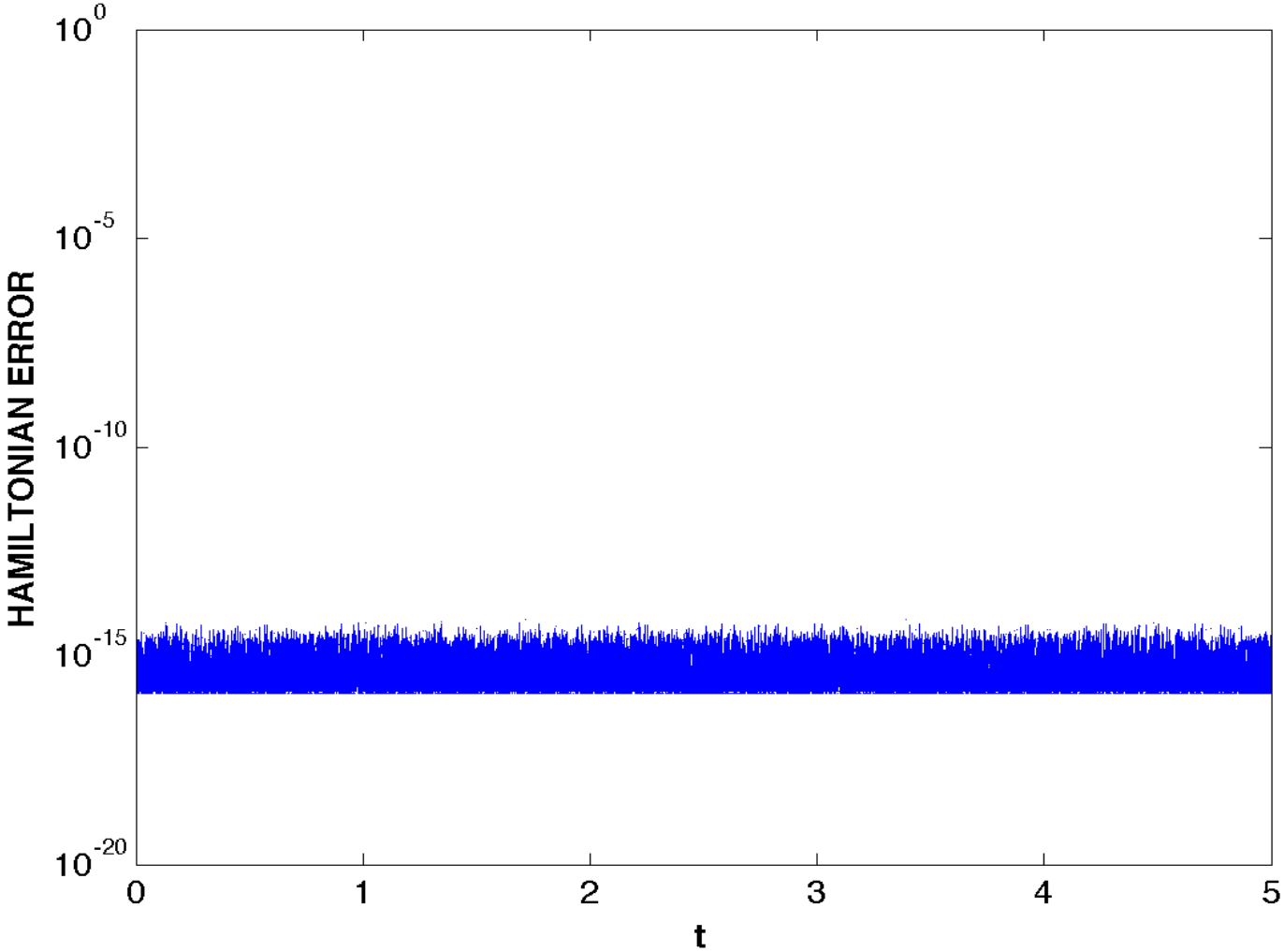
When $\alpha = 0$ one retrieves the 3-stage Gauss method.

68 - Second sixth-order EQUIP variant

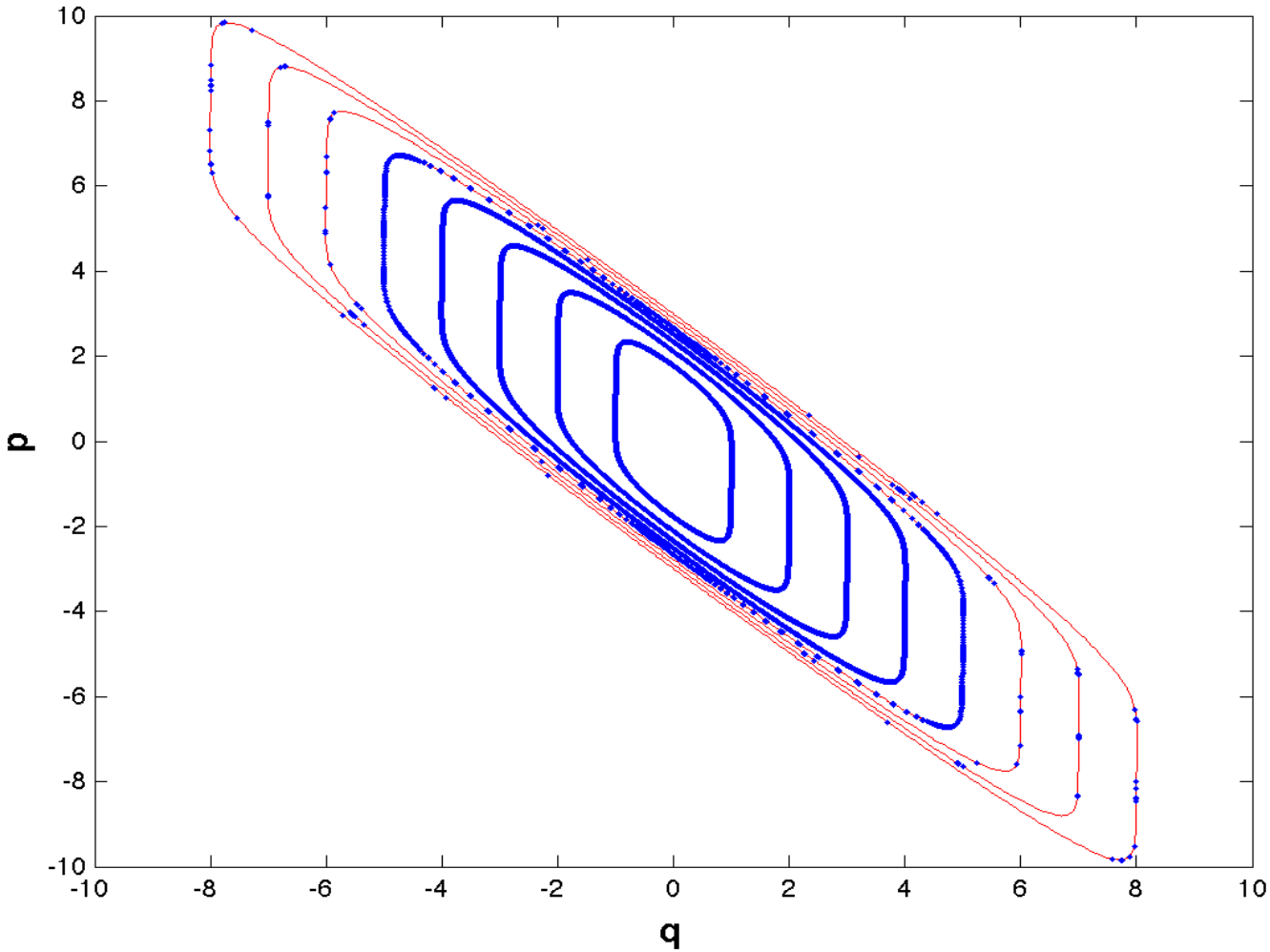
$$
\begin{array}{c|ccc}
\frac{1}{2}-\frac{\sqrt{15}}{10} & \frac{5}{36} & \frac{2}{9}-\frac{\sqrt{15}}{15}-\alpha\frac{2}{3} & \frac{5}{36}-\frac{\sqrt{15}}{30}+\alpha\frac{2}{3} \\
\frac{1}{2} & \frac{5}{36}+\frac{\sqrt{15}}{24}+\alpha\frac{5}{12} & \frac{2}{9} & \frac{5}{36}-\frac{\sqrt{15}}{24}-\alpha\frac{5}{12} \\
\frac{1}{2}+\frac{\sqrt{15}}{10} & \frac{5}{36}+\frac{\sqrt{15}}{30}-\alpha\frac{2}{3} & \frac{2}{9}+\frac{\sqrt{15}}{15}+\alpha\frac{2}{3} & \frac{5}{36} \\
\hline
 & \frac{5}{18} & \frac{4}{9} & \frac{5}{18}
\end{array}
$$

Also in this case, when $\alpha = 0$ one retrieves the 3-stage Gauss method.

69 - EQUIP(2), $h = 10^{-3}$



70 - EQUIP(2), $h = 10^{-3}$



71 - Conclusions

- Matrix formulation of Runge-Kutta methods constitutes a powerful framework for Geometric Integration;
- Energy-conserving HBVM(k,s) Runge-Kutta methods can be efficiently analyzed in this framework, as well as their efficient implementation;
- The larger class of Line Integral Methods can be obtained as a straightforward generalization;
- Low-rank symplectic Runge-Kutta methods are also easily derived within this framework;
- Energy and QUadratic Invariants Preserving methods can be derived, thus providing a further direction of investigation.

Hippocrates platanus

Hippocrates-Wannerus platanus

Happy birthday, Gerhard!