

Splitting methods and energy preservation for separable Hamiltonians

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Splitting Methods for Differential Equations
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- Energy-preservation vs symplecticity
- Energy-preserving methods:
 - ▶ The Average Vector Field (AVF) method
 - ▶ Extended collocation methods (for polynomial Hamiltonians)
 - ▶ Energy-preserving variant of collocation methods
 - ▶ B-series methods
- Explicit symplectic methods:
 - ▶ Splitting and composition schemes as explicit, symplectic, partitioned Runge-Kutta methods
 - ▶ Order conditions of ESPRK schemes
 - ▶ One-parameter families of order two and four
 - ▶ Minimum energy error methods
 - ▶ Examples of energy preservation

Energy-preservation vs symplecticity

We consider the numerical integration of (autonomous) Hamiltonian systems

$$\dot{y} = J^{-1} \nabla H(y), \quad J = \begin{pmatrix} 0 & -I \\ I & 0 \end{pmatrix},$$

where the Hamiltonian function $H(y)$ is assumed to be sufficiently differentiable.

Main properties: Energy-preservation AND symplecticity of the flow ($\varphi_t(y_0) = y(t)$, if $y(0) = y_0$)

$$\dot{H} = 0,$$

$$\varphi_t'^T J \varphi_t' = J.$$

Looking for: symplectic AND energy-preserving integrators $y_{n+1} = \Phi_h(y_n)$ satisfying both the following properties:

- the one-step map $\Phi_h(y_n)$ is symplectic (the Jacobian matrix satisfies $\Phi_h'(y_n)^T J \Phi_h'(y_n) = J$),
- $H(y_{n+1}) = H(y_n)$ for all n and $h > 0$.

No chance: Symplectic integrators, in general, do not exactly conserve the Hamiltonian.

Backward error analysis

Symplectic one-step methods **nearly conserve** the Hamiltonian (of an arbitrary system) over exponentially long times. The sequence $H(y_n)$ displays an oscillating behavior and the amplitude of oscillation is bounded with respect to the time and of size $\mathcal{O}(h^p)$.

Störmer/Verlet scheme

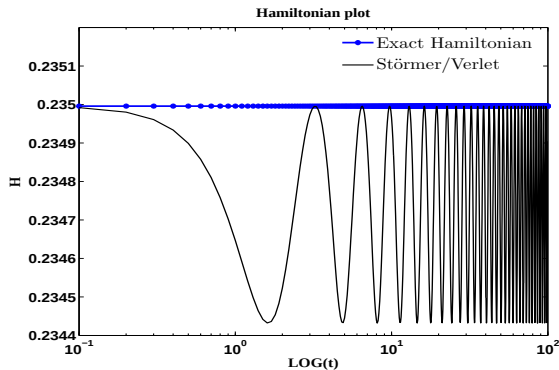


Figure: Energy function $H_4(p_n, q_n) = \frac{1}{2}p_n^2 + \frac{1}{2}q_n^2 - \frac{1}{24}q_n^4$, $h = 0.1$, $t = [0, 100]$, $[q_0, p_0] = [0.7, 0]$

Implicit Midpoint Rule (1-stage, Gauss method)

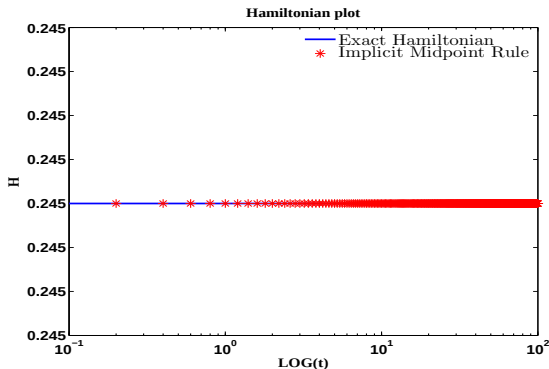


Figure: Energy function $H_2(p_n, q_n) = \frac{1}{2}p_n^2 + \frac{1}{2}q_n^2$, $h = 0.1$, $t = [0, 100]$, $[q_0, p_0] = [0.7, 0]$

Symplectic RK methods conserve quadratic Hamiltonian functions:

$$H(y) = \frac{1}{2}y^T Cy$$

but fail to yield conservation for higher degrees.

Symplectic B-series methods preserve quadratic invariants.

P. Chartier, E. Faou, A. Murua, Numer. Math. 103, 2006.

However, in general, symplecticity does not guarantee the preservation of the energy!

Energy-preserving methods

A few years ago, the unfruitful attempts to devise energy-preserving RK methods culminated in the general feeling that they should be symplectic and they could not preserve polynomial Hamiltonians of degree higher than two.

(A. Iserles and A. Zanna, Preserving algebraic invariants with Runge-Kutta methods, *J. Comput. Appl. Math.*, **125**, 2000, 69–81).

Average Vector Field integrator

The AVF method is defined as

$$y_{n+1} = y_n + h \int_0^1 J^{-1} \nabla H(\xi y_{n+1} + (1 - \xi) y_n) d\xi$$

- **Main property:** Energy preservation in Hamiltonian system.
- R.I McLachlan, G.R.W. Quispel, N. Robidoux, J.R. Soc. Lond. Philos. Trans. Ser. A Math. Phys. Eng. Sci. 1999.
- G.R.W. Quispel, D.I. McLaren, J.Phys. A: Math. Theor. 41, 2008.

Proof

Let $\sigma(\xi) = \xi y_{n+1} + (1 - \xi)y_n$ the segment joining y_n and y_{n+1} , with $\xi \in [0, 1]$ then

$$\begin{aligned} H(y_{n+1}) - H(y_n) &= \int_{\sigma} \nabla H(z) dz = \\ &= \int_0^1 \nabla H(\sigma(\xi))^T \dot{\sigma}(\xi) d\xi = \\ &= \int_0^1 \nabla H(\sigma(\xi))^T (y_{n+1} - y_n) d\xi = \\ &= h \int_0^1 \nabla H(\sigma(\xi))^T d\xi \int_0^1 J^{-1} \nabla H(\sigma(\xi)) d\xi = 0. \end{aligned}$$

Polynomial Hamiltonians

Consider polynomial Hamiltonian functions, then the integral appearing in the AVF method can be exactly replaced by a suitable quadrature formula.

For example, suppose H quadratic, then the 2-stages Lobatto quadrature formula leads to

$$y_{n+1} - y_n = h \frac{1}{2} J^{-1} (\nabla H(y_n) + \nabla H(y_{n+1}))$$

that is the Trapezoidal method (not symplectic).

Similarly, 1-stage Gauss method leads to

$$y_{n+1} - y_n = h J^{-1} \left(\nabla H\left(\frac{1}{2}(y_n + y_{n+1})\right) \right)$$

that is the Implicit Midpoint method (symplectic: no surprise since H is quadratic).

The Discrete Average Vector Field integrators

The DAVF method is defined as

$$y_{n+1} = y_n + h \sum_{i=1}^s b_i J^{-1} \nabla H(c_i y_{n+1} + (1 - c_i) y_n)$$

where b_i and c_i are weights and knots of a quadrature formula of degree m .

It is a Runge-Kutta method with Butcher tableau $A = cb^T$.

- Main property: Energy preservation for polynomial Hamiltonians of degree $m + 1$.

Proof, again

Let $\sigma(c) = cy_{n+1} + (1 - c)y_n$ the segment joining y_n and y_{n+1} , with $c \in [0, 1]$ then

$$H(y_{n+1}) - H(y_n) = \int_{\sigma} \nabla H(z) dz =$$

$$\int_0^1 \nabla H(\sigma(c))^T \dot{\sigma}(c) dc = \int_0^1 \nabla H(\sigma(c))^T (y_{n+1} - y_n) dc =$$

$$h \int_0^1 \nabla H(\sigma(c))^T dc \sum_{i=1}^s b_i J^{-1} \nabla H(\sigma(c_i)) =$$

$$h \sum_{j=1}^s b_j \nabla H(\sigma(c_j))^T \sum_{i=1}^s b_i J^{-1} \nabla H(\sigma(c_i)) = 0$$

Example: DAVF 2-steps Radau IIA: exact on polynomials of second degree

$$y_{n+1} - y_n = J^{-1} \left(\frac{3}{4} \nabla H(Y_{1/3}) + \frac{1}{4} \nabla H(Y_1) \right), \quad Y_{1/3} = \frac{1}{3} y_{n+1} + \frac{2}{3} y_n, \quad Y_1 = y_{n+1},$$

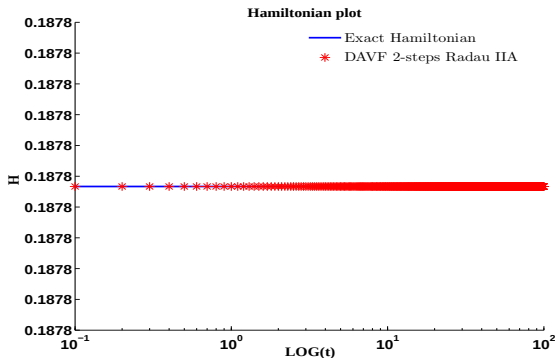


Figure: Energy function $H_3(p_n, q_n) = \frac{1}{2}p^2 + \frac{1}{2}q^2 - \frac{1}{6}q^3$, $h = 0.1$, $t = [0, 100]$, $[q_0, p_0] = [0.7, 0]$

REMARK

All these methods have only a second order accuracy...

Generalizations:

- Extended collocation methods (for polynomial Hamiltonian)
- Energy-preserving variant of collocation methods
- B-series methods

Extended collocation methods: sketch of the idea

Improve the order accuracy by

- increasing the degree of the polynomial curve $\sigma(c)$
- considering quadrature formula that takes into account the degree of $\nabla H(\sigma(c))^T \dot{\sigma}(c)$

With respect to classical collocation methods, extended collocation methods increase the number of inner stages for assuring the energy-preservation.

B. Pace. PhD thesis, 2008., F. Iavernaro, B. Pace., AIP Conf. Proc., 2007 and 2008, F. Iavernaro and D. Trigiante, JNAIAM 4, 2009.

Example: 5-stages extended Lobatto IIIA

- order 4
- energy-preservation of polynomial Hamiltonian of degree 3.

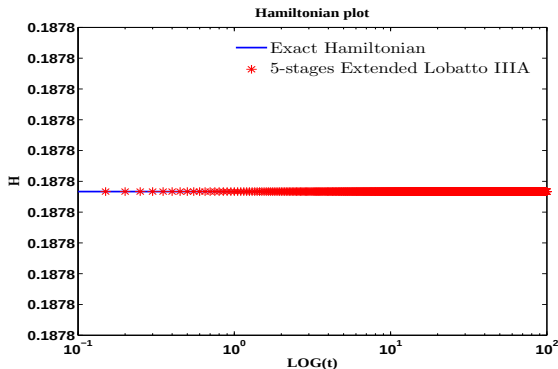


Figure: Energy function $H_3(p_n, q_n) = \frac{1}{2}p_n^2 + \frac{1}{2}q_n^2 - \frac{1}{6}q_n^3$, $h = 0.1$, $t = [0, 100]$, $[q_0, p_0] = [0.7, 0]$

Energy-preserving variant of collocation methods: sketch of the idea

- For generic Hamiltonian do not replace the integral by a quadrature formula,
- Consider the AVF method as a RK scheme with a continuum of stages lying on a straight line:

$$y_{n+1} = y_n + h \int_0^1 J^{-1} \nabla H(Y_\xi) d\xi,$$

$$Y_\xi = \xi y_{n+1} + (1 - \xi) y_n (\approx y(t_n + \xi h)),$$

- generalize to polynomial curves of degree $s > 1$.

E. Hairer, JNAIAM, 2010.

Example: 4-order energy-preserving collocation method

$$u(t_n + \xi h) = y_n + (y_{n+1} - y_n) \xi + 2(y_{n+1} - 2 Y_{1/2} + y_n) \xi (\xi - 1)$$

$$Y_{1/2} = y_n + h \int_0^1 \left(\frac{5}{4} - \frac{3}{2} \xi \right) J^{-1} \nabla H(u(t_n + \xi h)) d\xi$$

$$y_{n+1} = y_n + h \int_0^1 J^{-1} \nabla H(u(t_n + \xi h)) d\xi.$$

Remark: By approximating the integrals by 5 stages Lobatto quadrature rule we obtain the 5-stages extended Lobatto IIIA method.

B-series methods: sketch of the idea

Consider the AVF method as a B-series method that conserve energy in Hamiltonian system.

- Prove that AVF method is a B-series second-order method.
- Increase the order by considering compositions of AVF method with its adjoint.

E. Celledoni, R.I. McLachlan, D.I. McLaren, B.Owren, G.R.W. Quispel, W.M. Wright., ESAIM: M2AN 43, 2009.

Explicit symplectic integrators

We have seen that the energy-preserving methods are implicit and requires the evaluation of an exact integral (or a suitable approximation in case of polynomial Hamiltonians).

In case of separable Hamiltonians, we are giving up to use symplectic, explicit methods of minimum effective error.

- R.I. McLachlan, SIAM J. Sci. Comput., 16, 1995.
- S. Blanes, P.C. Moan, JCAM, 142, 2002.

Splitting methods as symplectic partitioned Runge-Kutta methods

Separable Hamiltonians $H(p, q) = T(p) + U(q)$: interpret H as the sum of two Hamiltonians $T(p)$ and $U(q)$ and solve exactly the corresponding Hamiltonian systems. If the flows of the two systems are denoted as φ_t^T and φ_t^U , then

$$\varphi_h^T \circ \varphi_h^U$$

is the **symplectic Euler method**. This is equivalent to the Runge Kutta partitioned method

$$\begin{array}{c|c} 0 & 0 \\ \hline & 1 \end{array} \quad \begin{array}{c|c} 1 & 1 \\ \hline & 1 \end{array}$$

applied to the Hamiltonian system with stepsize h (p variable implicit and q variable explicit).

$$\begin{aligned} \dot{q} &= T_p(p) \\ \dot{p} &= -U_q(q) \end{aligned}$$

More in general a splitting method with $2s + 1$ free parameters a_i and b_i ,

$$\varphi_{b_{s+1}h}^U \circ \varphi_{a_sh}^T \circ \cdots \circ \varphi_{b_2h}^U \circ \varphi_{a_1h}^T \circ \varphi_{b_1h}^U,$$

is equivalent to the following $s + 1$ stages PRK scheme

$$\begin{array}{c|cccc} c_1^{(a)} & 0 & & & \\ c_2^{(a)} & a_1 & 0 & & \\ c_3^{(a)} & a_1 & a_2 & 0 & \\ & \vdots & \vdots & \vdots & \ddots \\ c_{s+1}^{(a)} & a_1 & a_2 & \dots & a_s & 0 \\ \hline & a_1 & a_2 & \dots & \dots & 0 \end{array}$$

$$\begin{array}{c|ccccc} c_1^{(b)} & b_1 & & & & \\ c_2^{(b)} & b_1 & b_2 & & & \\ c_3^{(b)} & b_1 & b_2 & b_3 & & \\ & \vdots & \vdots & \vdots & \ddots & \\ c_{s+1}^{(b)} & b_1 & b_2 & b_3 & \dots & b_{s+1} \\ \hline & b_1 & b_2 & \dots & \dots & b_{s+1} \end{array}$$

Splitting methods are explicit, symplectic methods.

The simplicity of the method can be verified (also) via PRK theory:

- PRK schemes based on two k stages RK methods (a_{ij}, b_i, c_i) and $(\hat{a}_{ij}, \hat{b}_i, \hat{c}_i)$, applied on separable Hamiltonian, if they satisfy

$$b_i \hat{a}_{ij} + \hat{b}_j a_{ij} = b_i \hat{b}_j, \quad i, j = 1, \dots, k,$$

are symplectic.

This is our case.

Effective order of a splitting method

We consider as measure of the error of a p -order method the **effective error**

$$E_f = s \left(\sum_{i=1}^m C_i^2 \right)^{(1/2m)}$$

where C_i , for $i = 1, \dots, m$ are the determining order equations for achieving an accuracy up to order $p + 1$.

Determining order conditions: $C(\tau) = \Phi(\tau) - \frac{1}{\gamma(\tau)} = 0$

Table: Elementary weights and density function values up to order five

$\Phi(\tau)$	$\gamma(\tau)$	$\Phi(\tau)$	$\gamma(\tau)$
$\sum_{i=1}^{s+1} b_i$	1	$\sum_{i=1}^s a_i$	1
$\sum_i^{s+1} b_i c_i^{(a)}$	2	$\sum_i^{s+1} b_i (c_i^{(a)})^2$	3
$\sum_{i=1}^{s+1} \sum_{j=1}^{i-1} b_i a_j c_j^{(b)}$	6	$\sum_{i=1}^{s+1} \sum_{j=1}^{i-1} b_i a_j (c_j^{(b)})^2$	12
$\sum_{i=1}^{s+1} b_i (c_i^{(a)})^3$	4	$\sum_{i=1}^{s+1} \sum_{j=1}^{i-1} \sum_{k=1}^i b_i a_j b_k c_k^{(a)}$	24
$\sum_{i=1}^{s+1} b_i (c_i^{(a)})^4$	5	$\sum_{i=1}^{s+1} \sum_{j=1}^{i-1} \sum_{l=1}^j \sum_{k=1}^{l-1} b_i a_j b_l a_k c_k^{(b)}$	120
$\sum_{i=1}^{s+1} \sum_{j=1}^{i-1} \sum_{l=1}^j b_i c_i^{(a)} a_j b_l c_l^{(a)}$	30	$\sum_{i=1}^{s+1} \sum_{j=1}^{i-1} \sum_{l=1}^j b_i a_j b_l (c_l^{(a)})^2$	60
$\sum_{i=1}^{s+1} \sum_{j=1}^{i-1} \sum_{l=1}^j b_i a_j c_j^{(b)} b_l c_l^{(a)}$	40	$\sum_{i=1}^{s+1} \sum_{j=1}^{i-1} b_i a_j (c_j^{(b)})^3$	20

Symmetric methods

$$b_{s+2-i} = b_i, \quad i = 1, \dots, s+1, \quad a_{s+1-i} = a_i \quad i = 1, \dots, s.$$

- free parameters a_i and b_i reduce to $s+1$
- parameters that satisfy odd orders of accuracy p , automatically verify the conditions for the even order $p+1$.

For example, two conditions of the first order, assure the second order:

$$\sum_{i=1}^{s+1} b_i = 1, \quad \sum_{i=1}^s a_i = 1$$

It is enough to take $s = 1$, and solve $a_1 = 1$ and $2b_1 = 1$ with $b_1 = b_2$ to define the Störmer-Verlet scheme $\varphi_{h/2}^U \circ \varphi_h^T \circ \varphi_{h/2}^U$

One-parameter second-order methods

In order to preserve one degree of freedom, take $s = 2$ and solve the system

$$2b_1 + b_2 = 1, \quad 2a_1 = 1.$$

with respect to b_2 and a_1 considering $b = b_1$ as a free parameter. We obtain the class of second order methods defined as

$$\varphi_{bh}^U \circ \varphi_{h/2}^T \circ \varphi_{(1-2b)h}^U \circ \varphi_{h/2}^T \circ \varphi_{bh}^U$$

The effective error is given by

$$E_f(b) = \sqrt[4]{4b^4 - 8b^3 + 19/3b^2 - 5/3b + 5/36}$$

By setting $y = \sqrt[3]{36 + 2\sqrt{326}}$, it achieves its minimum value at

$$b_{opt\ ML} = \frac{2 + 6y - y^2}{12y} \approx 0.1932 \text{ (MLS}_2 \text{ scheme)}.$$

Second-order methods with minimum error in energy

Instead of minimizing the effective error, search for the values of $b = b_n$ which **minimizes the error on energy**, at each timestep t_n .

Starting from y_0 at $t_0 = 0$, the method at $t_n = n h$, searches for

$$\min_{b_n} |H(y_{n+1}) - H(y_0)|$$

with

$$y_{n+1} = \psi_h^{(n)}(y_n), \quad \psi_h^{(n)} = \varphi_{b_n h}^U \circ \varphi_{h/2}^T \circ \varphi_{(1-2b_n)h}^U \circ \varphi_{h/2}^T \circ \varphi_{b_n h}^U$$

Remark

- Provided that, for each n , there exists a minimum equal to zero, the method gives a second-order, energy-preserving integrator.
- If not, the method provides a second-order integrator with minimum error in energy.
- From a computational point of view it requires, for each n , the search for a zero of a scalar function with respect to a scalar variable.

Example: linear oscillator

$$\dot{y} = J^{-1} \nabla H(y), \quad H(y) = \frac{y^T y}{2}, \quad y \in \mathbb{R}^2.$$

Evaluate the numerical solution as

$$y_1 = \psi_h^{(0)}(y_0) = K(b_1, h)y_0.$$

with

$$K(b_1, h) = \frac{1}{8} \begin{bmatrix} p(b_1, h) & e(b_1, h) + q(b_1, h) \\ e(b_1, h) - q(b_1, h) & p(b_1, h) \end{bmatrix}$$

$$\begin{aligned} p &= p(b_1, h) &= 8 - 4h^2 + 2h^4 b_1 - 4h^4 b_1^2 \\ e &= e(b_1, h) &= h^3(2h^2 b_1^3 - (4 + h^2)b_1^2 + 6b_1 - 1) \\ q &= q(b_1, h) &= h(8 - h^2) - 2h^3 b_1 + h^3(4 + h^2)b_1^2 - 2h^5 b_1^3 \end{aligned}$$

with

$$\det(K) - 1 = p^2 + q^2 - e^2 - 64 = 0$$

Evaluate

$$H(y_1) - H(y_0) = \frac{1}{2} y_0^T (K^T K - I) y_0$$

with

$$K^T K = \frac{1}{64} \begin{bmatrix} p^2 + (e - q)^2 & 2 p e \\ 2 p e & p^2 + (e + q)^2 \end{bmatrix}.$$

Seek for solutions of $H(y_1) - H(y_0) = 0$ which do not depend on y_0 ;

it is easy to see that it is enough to find the (real) roots of the third order polynomial e since, from $\det(K) = 1$, it follows that $p^2 + q^2 - 64 = 0$.

Theorem Set $h > 0$ and let b_r a real root of the third order polynomial

$$e(b, h) = 2h^2 b^3 - (4 + h^2) b^2 + 6b - 1,$$

then, the scheme

$$\varphi_{b_r h}^U \circ \varphi_{h/2}^T \circ \varphi_{(1-2b_r)h}^U \circ \varphi_{h/2}^T \circ \varphi_{b_r}^U$$

is an **explicit, symplectic, energy preserving, second order scheme for the linear oscillator**

$$\dot{q} = p, \quad \dot{p} = -q$$

.

What about the efficiency? Plot the real roots of $e(b, h)$ for $h \in]0, 1]$.

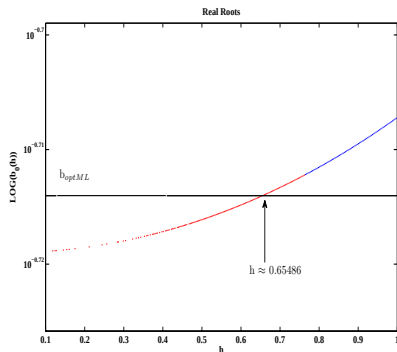
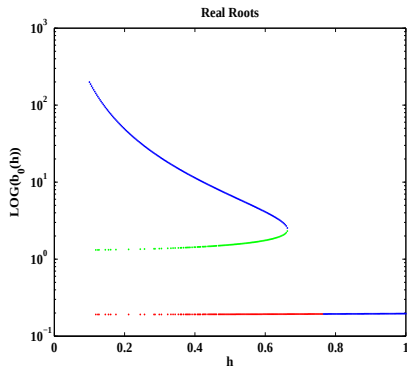


Figure: Real roots of $e(b, h)$ for $h \in]0, 1]$,

It turns out that, by choosing b^* as the real root which satisfies

$$\min_{b_r} |b_r - b_{opt\ ML}| = |b^* - b_{opt\ ML}|$$

we find **the optimal energy-preserving (symmetric) second order scheme (EPS₂).**

Moreover, for value of $h \approx 0.65486$ the MLS₂ and EPS₂ schemes coincide, hence MLS₂ scheme behaves as an energy-preserving scheme for the linear oscillator.

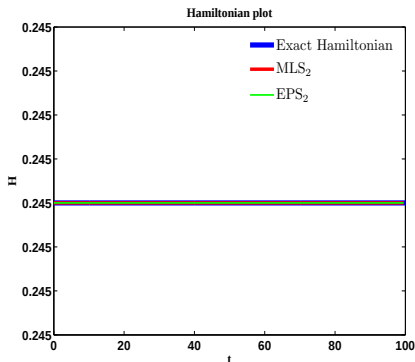
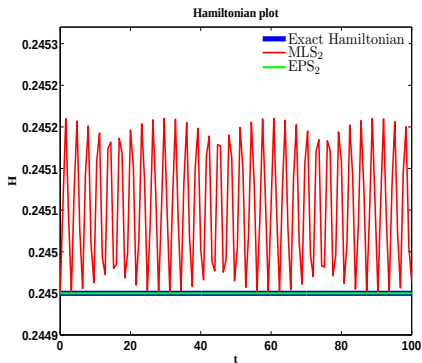


Figure: Energy function $H_2(q_n, p_n) = \frac{1}{2}p_n^2 + \frac{1}{2}q_n^2$, $t = [0, 100]$, $[q_0, p_0] = [0.7, 0]$, $h = 0.8$ (left) and $h = 0.6548603813333458$ (right)

Higher-order polynomial Hamiltonians

Suppose $H(p, q) = 1/2p^2 + \sum_{i=0}^{s_q} b_i q^i$, $s_q \geq 3$, $s_q \in \mathcal{N}$.

- The degree of the polynomial $H(p_{n+1}, q_{n+1}) - H(p_n, q_n)$, with respect to b_n , is $2(s_q^2 - s_q + 1)$.
- The roots will depend also on p_n and q_n and the symplecticity can be lost.
- Real roots may not exist.

It is not possible to develop the analysis done on the linear oscillator...

Let us use an algorithm for finding a minimum of nonlinear scalar functions.

The values $b_n = b_{opt\ ML}$ will be the starting guesses for our method, for each n .

The accuracy of the optimization algorithm plays a crucial role.

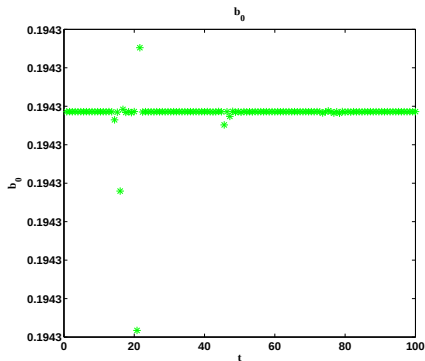
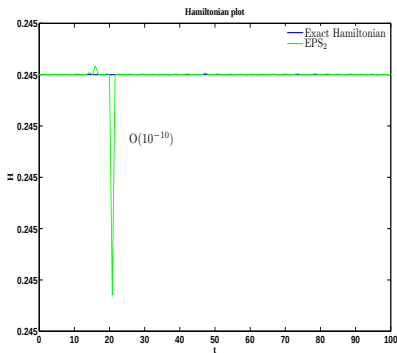


Figure: Use `fsolve` Matlab built in function. Energy function

$H_2(p_n, q_n) = \frac{1}{2}p_n^2 + \frac{1}{2}q_n^2$, $h = 0.8$, $t = [0, 100]$, $[q_0, p_0] = [0.7, 0]$ (left) and values b_n (right).

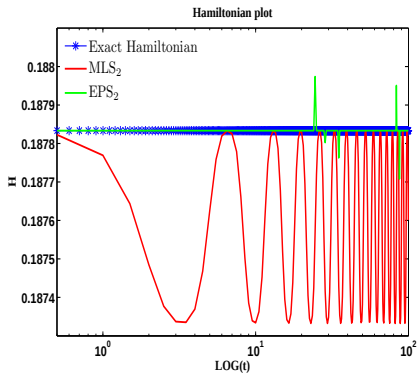
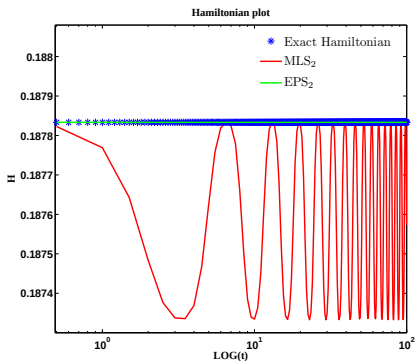


Figure: Energy function $H_3(p_n, q_n) = \frac{1}{2}p_n^2 + \frac{1}{2}q_n^2 - \frac{1}{6}q_n^3$, $t = [0, 100]$, $h = 0.5$, $[q_0, p_0] = [0.7, 0]$ (left: exact, right: use fsolve)

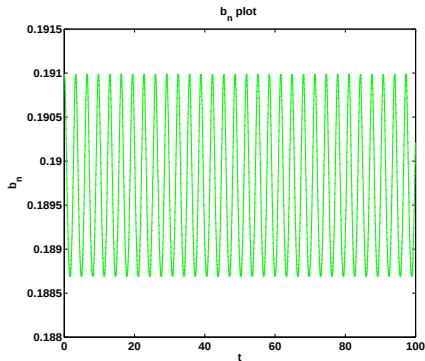
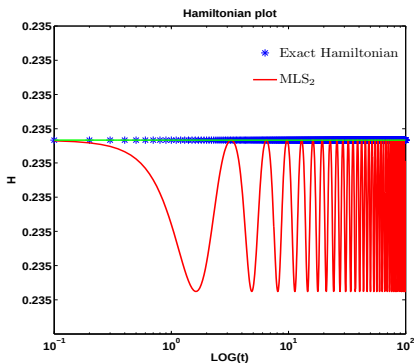


Figure: Energy function $H_4(p_n, q_n) = \frac{1}{2}p_n^2 + \frac{1}{2}q_n^2 - \frac{1}{24}q_n^4$, $h = 0.1$, $t = [0, 100]$, $[q_0, p_0] = [0.7, 0]$ (left) and values b_n (right)

For polynomial Hamiltonians considered, the proposed method behaves as

second-order energy-preserving integrators.

What happens for general non linear Hamiltonians?

An example: Perturbed Kepler problem

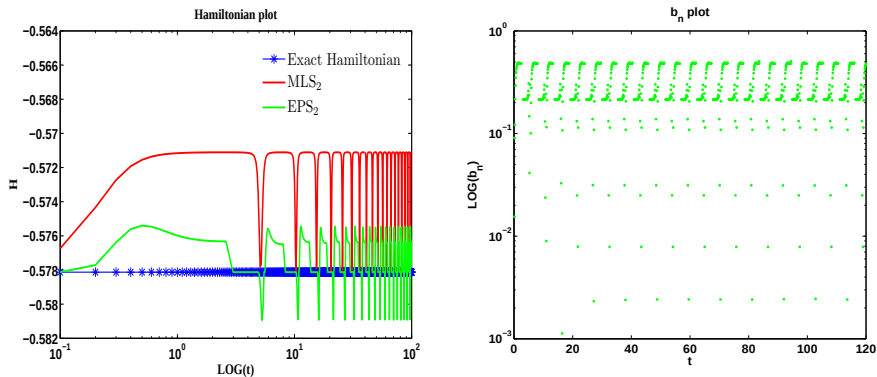


Figure: Energy function $H(q_n, p_n) = \frac{1}{2} p_n^T p_n - \frac{1}{\|q_n\|_2} - \frac{\epsilon}{3\|q_n\|_2^3}$, $\epsilon = 0.015$, $h = 0.1$,
 $t = [0, 120]$, $q_0 = [1 - e, 0]$, $p_0 = [0, \sqrt{\frac{1+e}{1-e}}]$, $e = 0.6$

For the considered non linear Hamiltonian problem, the proposed method behaves as a **second-order integrators with minimum error in energy preservation.**

Let us increase the order.

Fourth-order methods with minimum error in energy

Two additional conditions:

$$\sum_i^{s+1} b_i (c_i^{(a)})^2 - \frac{1}{3} = 0, \quad \sum_{i=1}^{s+1} \sum_{j=1}^{i-1} b_i a_j c_j^{(b)} - \frac{1}{6} = 0.$$

By setting $s = 4$ we obtain two families of fourth-order methods depending on one parameter a_n .

$$\varphi_{b_1(a_n)h}^U \circ \varphi_{a_nh}^T \circ \varphi_{b_2(a_n)h}^U \circ \varphi_{\frac{1-2a_n}{2}h}^T \circ \varphi_{(1-2(b_1(a_n)+b_2(n)))h}^U \circ \varphi_{\frac{1-2a_n}{2}h}^T \circ \varphi_{b_2(a_n)h}^U \circ \varphi_{a_nh}^T \circ \varphi_{b_1(a_n)h}^U$$

where $a_n > 1/2$, $a_n \neq \frac{1+\sqrt{5}}{4} \approx 0.809$ and

$$\begin{aligned} b_1(a_n) &= \frac{(24a_n^3 - 20a_n^2 + 2a_n \pm \sqrt{2}\alpha(1-2a_n))}{12a_n(4a_n^2 - 2a_n - 1)} \\ b_2(a_n) &= \frac{(-4a_n + 8a_n^2 \mp \sqrt{2}\alpha)}{-12a_n(1 + 8a_n^3 - 8a_n^2)}; \end{aligned}$$

with $\alpha = \alpha(a_n) = \sqrt{a_n(8a_n - 24a_n^2 + 24a_n^3 - 1)}$.

The optimal one-parameter fourth order splitting method in the second family (MLS₄) is achieved in correspondence of $a_n = a_{optML} \approx 0.5532$.

Linear oscillator

Again, the numerical solution can be expressed as

$$y_1 = \psi_h^{(0)}(y_0) = K(a_1, h)y_0.$$

with

$$K(a_1, h) = \begin{bmatrix} p(a_1, h) & e(a_1, h) + q(a_1, h) \\ e(a_1, h) - q(a_1, h) & p(a_1, h) \end{bmatrix}.$$

Unfortunately, $e(a_1, h)$ shows a not-polynomial dependence a_1 due to presence of $\alpha(a_1)$.

Choose the second family of methods

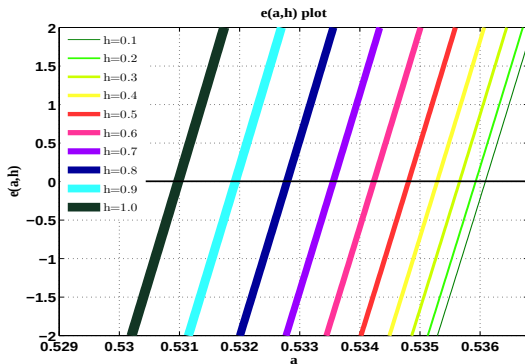


Figure: $e(a, h)$, for different values of h

For values of $h \rightarrow 0$, $e(a, h) = 0$ for $a \approx 0.5361$.

Theorem Set $h > 0$ and denote with a_r the (real) zero of the function $e(a, h)$ for $\frac{1}{2} < a < \frac{1+\sqrt{5}}{4}$ then, the scheme

$$\varphi_{b_1(a_r)h}^U \circ \varphi_{a_r h}^T \circ \varphi_{b_2(a_r)h}^U \circ \varphi_{\frac{1-2a_r}{2}h}^T \circ \varphi_{(1-2(b_1(a_r)+b_2(a_r)))h}^U \circ \varphi_{\frac{1-2a_r}{2}h}^T \circ \varphi_{b_2(a_r)h}^U \circ \varphi_{a_r h}^T \circ \varphi_{b_1(a_r)h}^U$$

is an **explicit, symplectic, energy preserving, fourth order scheme for the linear oscillator**

$$\dot{q} = p, \quad \dot{p} = -q.$$

Notice that the accuracy increases for decreasing values of h . Differently from the second order method, this scheme cannot assume the optimal value related to $a = a_{optML} \approx 0.5532$.

Linear oscillator

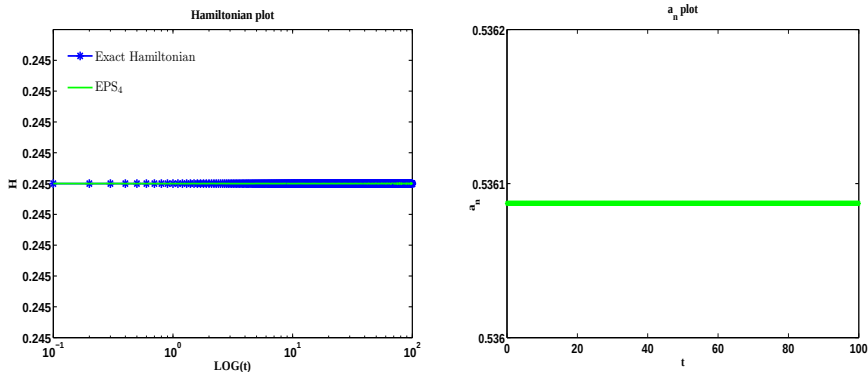


Figure: Energy function $H_2(p_n, q_n) = \frac{1}{2}p_n^2 + \frac{1}{2}q_n^2$, $h = 0.1$, $t = [0, 100]$, $[q_0, p_0] = [0.7, 0]$

Higher degree polynomials: cubic Hamiltonian

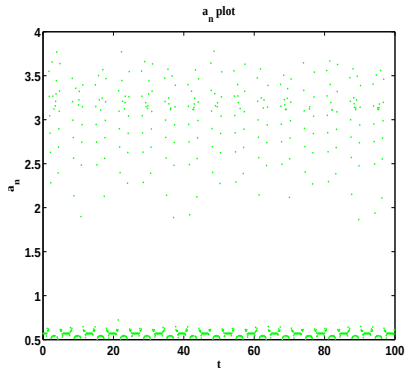
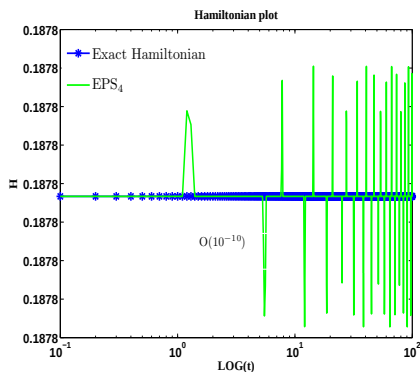


Figure: Energy function $H_3(p_n, q_n) = \frac{1}{2}p_n^2 + \frac{1}{2}q_n^2 - \frac{1}{6}q_n^3$, $t = [0, 100]$, $h = 0.5$, $[q_0, p_0] = [0.7, 0]$

Quartic Hamiltonian

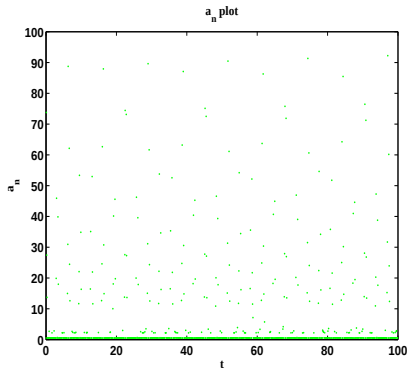
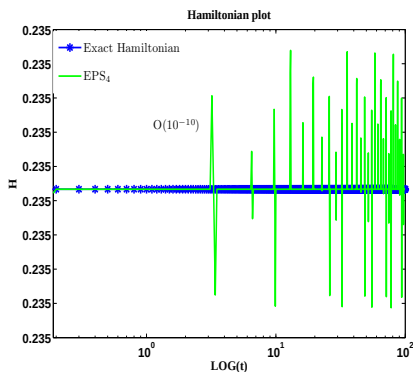


Figure: Energy function $H_4(p_n, q_n) = \frac{1}{2}p_n^2 + \frac{1}{2}q_n^2 - \frac{1}{24}q_n^4$, $h = 0.1$, $t = [0, 100]$, $[q_0, p_0] = [0.7, 0]$ (left) and values b_n (right)

Perturbed Kepler problem

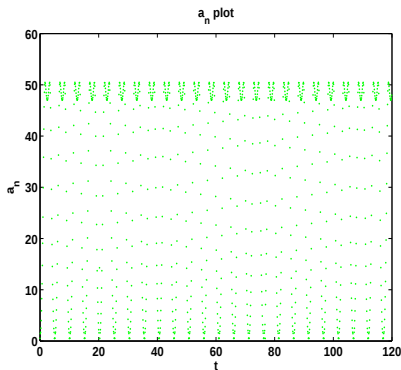
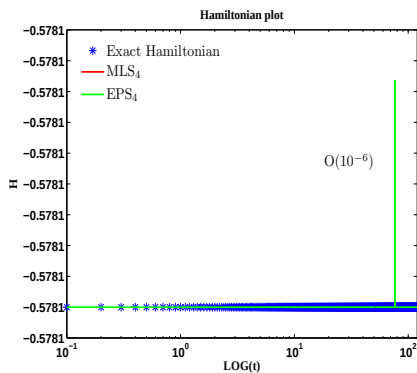


Figure: Energy function $H(q_n, p_n) = \frac{1}{2} p_n^T p_n - \frac{1}{\|q_n\|_2} - \frac{\epsilon}{3\|q_n\|_2^3}$, $\epsilon = 0.015$, $h = 0.1$,
 $t = [0, 100]$, $q_0 = [1 - e, 0]$, $p_0 = [0, \sqrt{\frac{1+e}{1-e}}]$, $e = 0.6$

CONCLUSIONS

- We propose second and fourth order splitting schemes for separable Hamiltonians featured by minimum error in energy preservation.
- In case of the linear oscillator they are explicit, symplectic, energy-preserving integrators.
- In case of polynomial Hamiltonians the schemes (seems to) behave as energy-preserving methods, in the general case they are methods with minimum error in energy. However, an efficient optimization algorithm is required.
- Energy-preserving methods with complex coefficients, higher order methods as well as the generalization to non-separable Hamiltonians will be the subject of our future research.

Thanks to all for your attention!