Collocation-like methods with conservation properties for the numerical integration of Hamiltonian systems

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MAIN TOPIC

TO INTRODUCE A FAMILY OF RUNGE KUTTA METHODS OF ARBITRARILY HIGH ORDER WITH ENERGY PRESERVING PROPERTIES

AND

TO HIGHLIGHT ITS RELATIONSHIP WITH COLLOCATION METHODS

DEFINITION OF THE PROBLEM

We consider the numerical integration of Hamiltonian systems

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

The vector state y is made up of:

$$y = \begin{pmatrix} q \\ p \end{pmatrix} \begin{array}{l} \rightarrow \text{generalized coordinates} \\ \rightarrow \text{conjugate momenta} \end{array}$$

ASSUMPTION: the Hamiltonian function $H(y) = H(p, q)$ is a polynomial in the variables p and q.

AIM: To define one-step methods that conserve the Hamiltonian function:

$$H(y_{n+1}) = H(y_n) \quad \text{for all } n \text{ and } h > 0$$

MOTIVATIONS (1/2)

- Many interesting Hamiltonian systems arising from different fields of study are defined by polynomial Hamiltonian functions.

Example: Fermi-Pasta-Ulam Problem

This problem describes the interaction of $2m$ mass points linked with alternating soft nonlinear and stiff linear springs, in a one-dimensional lattice with fixed end points ($q_0 = q_{2m+1} = 0$). The Hamiltonian function is

$$H(p,q) = \frac{1}{2}\sum_{i=1}^{m}(p_{2i-1}^2 + p_{2i}^2) + \frac{\omega^2}{4}\sum_{i=1}^{m}(q_{2i} - q_{2i-1})^2 + \sum_{i=0}^{m}(q_{2i+1} - q_{2i})^4.$$

In our experiments we chose the stiff parameter $\omega = 50$.

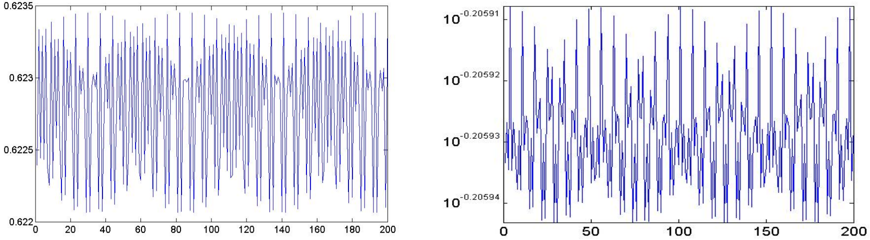
MOTOVATIONS (2/2)

It is well known that symplectic RK-methods only conserve quadratic Hamiltonian functions:

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

but, in general, they fail to yield conservation for higher degree. So do symmetric methods.

COUNTEREXAMPLES (1/2)

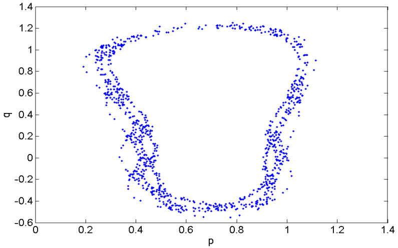


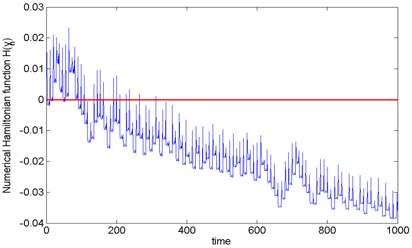
Energy function evaluated over the numerical solution obtained by solving the quartic pendulum equation

$$H(p, q) = \frac{1}{2}p^2 + \frac{1}{2}q^2 - \frac{1}{24}q^4.$$

by the Lobatto IIIA method of order four (left picture) and Gauss method of order six (right picture).

COUNTEREXAMPLES (2/2)





Even worse, the discrete energy function $H(p_n, q_n)$ may undergo a drift (even if the method is selected to be symmetric). LobattoIIIB order 4, $h = 1; y0 = [1, 0]$

$$H(p, q) = \frac{1}{3}p^3 - \frac{1}{2}p + \frac{1}{30}q^6 + \frac{1}{4}q^4 - \frac{1}{3}q^3 + \frac{1}{6}.$$

- E. Faou, E. Hairer and T.-L. Pham, *Energy conservation with non-symplectic methods: Examples and counter-examples*, BIT 44, no. 4 (2004)

THE LINE INTEGRAL: THE KEY TOOL

Given a path $\sigma = c \in [0,1] \to \mathbb{R}^{2m}$ joining the points y_0 and y_1 in the phase space, we consider the line integral

$$\int_{y_0 \to y_1} \nabla H(y) dy \equiv \int_0^1 \dot{\sigma}(c)^T \nabla H(\sigma(c))\, dc$$

Due to conservativeness of the vector field, such integral is equal to $H(y_1) - H(y_0)$, no matter how $\sigma(c)$ is chosen.

The fundamental property we will consider is

$$\sigma(c) \equiv \underbrace{y(t_0 + ch)}_{\text{Exact solution}} \Longrightarrow H(y(t_0 + h)) = H(t_0)$$

which means Energy Conservation.

AIM

- To define a discrete counterpart of the line integral and
- to reproduce the energy conservation property when the continuous theoretical solution $y(t_0 + ch)$ is replaced by the numerical solution obtained by a suitable one-step method $y_1 = \Phi_h(y_0)$

SKETCH OF THE IDEA: quadratic Hamiltonian (1/2)

We consider one of the simplest RK methods: the trapezoidal method:

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

Multiplication of both sides by $\left(\nabla H(y_n) + \nabla H(y_{n+1}) \right)^T$ yields

$$\left(\nabla H(y_n) + \nabla H(y_{n+1}) \right)^T (y_{n+1} - y_n) = 0$$

CLAIM: For quadratic Hamiltonian functions this is tantamount to the conservation law:

$$H(y_{n+1}) = H(y_n), \text{ for all times } t_n$$

SKETCH OF THE IDEA: quadratic Hamiltonian (2/2)

PROOF: Consider the segment σ joining y_n to y_{n+1}

$$\sigma(t_0 + ch) = (1-c)y_n + cy_{n+1}, \text{ whith } c \in [0,1].$$

and the line integral

$$\begin{aligned} H(y_{n+1}) - H(y_n) &= \int_{y_n \to y_{n+1}} \nabla H(y) dy = \int_0^1 \dot{\sigma}(t_0 + ch)^T \nabla H(\sigma(t_0 + ch))\, dc \\ &= h(y_{n+1} - y_n)^T \int_0^1 \nabla H(\sigma(t_0 + ch))\, dc \\ &= \frac{1}{2} h(y_{n+1} - y_n)^T (\nabla H(y_n) + \nabla H(y_{n+1})) \\ &= 0 \end{aligned}$$

$\nabla H(y)$ being linear.

How to generalize when $\deg H(y) = \nu$, for some $\nu \geq 2$?

Again, $\sigma(t_0 + ch) = (1-c)y_n + cy_{n+1}$, whith $c \in [0,1]$:

$$H(y_{n+1}) - H(y_n) = \int_{y_n \to y_{n+1}} \nabla H(y) dy = \int_0^1 \dot\sigma(t_0 + ch)^T \nabla H(\sigma(t_0 + ch))\, dc$$

$$= h(y_{n+1} - y_n)^T \int_0^1 \underbrace{\nabla H(\sigma(c))}_{\text{degree } \nu - 1}\, dc$$

$$= h(y_{n+1} - y_n)^T \underbrace{\sum_{i=1}^{k} b_i \nabla H(Y_i)}_{\substack{\text{quadrature formula with} \\ \text{degree of precision} \geq \nu - 1}}$$

- $Y_i = \sigma(t_0 + c_i h), \; i = 1, \ldots, k$
- $c_1, c_2, \ldots, c_k$ distinct abscissae in $[0,1]$.

Energy Preserving methods of order 2 (F.I.-B.Pace [2007])

$$
\begin{aligned}
y_{n+1} &= y_n + h\sum_{i=1}^{k} b_i f(Y_i), \\
Y_i &= (1-c_i)y_n + c_i y_{n+1}, \quad i = 1,\ldots,k
\end{aligned}
$$

Y_i are called *silent stages* since their presence does not affect the nonlinearity of the resulting R-K method: they are mono-implicit methods.

abscissae distribution	Energy preserving when
Newton-Cotes distribution	$\deg H \le k, k+1$
Lobatto distribution	$\deg H \le 2k-2$
Gauss distribution	$\deg H \le 2k$

A couple of examples (uniform distribution)

When $k = 2$ we obtain the trapezoidal method; for $k = 3$ and $k = 5$ we obtain respectively the methods:

$$y_{n+1} = y_n + \frac{h}{6}\left(f(y_n) + 4f(\frac{y_n + y_{n+1}}{2}) + f(y_{n+1})\right)$$

and

$$y_{n+1} = y_n + \frac{h}{90}\left(7f(y_n) + 32f(\frac{3y_n + y_{n+1}}{4}) + 12f(\frac{y_n + y_{n+1}}{2}) + 32f(\frac{y_n + 3y_{n+1}}{4}) + 7f(y_{n+1})\right)$$

When applied to $y' = f(t)$, these become the Newton-Cotes quadrature formulae of order 4 and 6 respectively.
On the other hand, when applied to general ODE problems their order reduces to two.

The Butcher tableau

The Butcher tableau associated with these methods is:

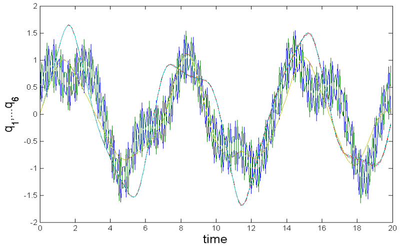
$$
\begin{array}{c|ccccc}
c_1 & c_1 b_1 & c_1 b_2 & \dots & \dots & c_1 b_k \\
c_2 & c_2 b_1 & c_2 b_2 & \dots & \dots & c_2 b_k \\
\vdots & \vdots & \vdots & & & \vdots \\
c_{s-1} & c_{s-1} b_1 & c_{s-1} b_2 & \dots & \dots & c_{s-1} b_s k \\
c_s & b_1 & b_2 & \dots & \dots & b_k \\
\hline
 & c_s b_1 & c_s b_2 & \dots & \dots & c_k b_k
\end{array}
=
\begin{array}{c|c}
c & cb^T \\
\hline
 & b^T
\end{array}
$$

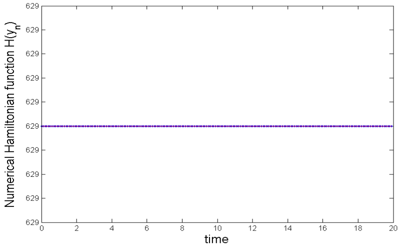
It is easily seen that each method under consideration has order two and is symmetric.

NUMERICAL TEST: Fermi-Pasta-Ulam Problem

$$H(q,p)=\frac{1}{2}\sum_{i=1}^{m}(p_{2i-1}^2+p_{2i}^2)+\frac{\omega^2}{4}\sum_{i=1}^{m}(q_{2i}-q_{2i-1})^2+\sum_{i=0}^{m}(q_{2i+1}-q_{2i})^4.$$

We chose $m=3$ (6 degrees of freedom) and $\omega=50$.



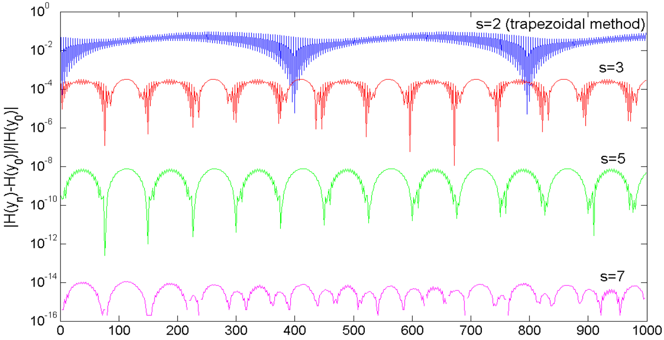


Stepsize $h=0.1$

NUMERICAL TEST: The pendulum equation

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

Parameters: interval $[0, 1e3]$, $h = 1$, $[q_0, p_0] = [\pi/2,\ 1/2]$



Increasing the number of silent stages results in a significant reduction of the error, independently of the choice of the stepsize h $\Longrightarrow$ PRACTICAL ENERGY CONSERVATION.

REMARK

- $H(y)$ a polynomial. If k is sufficiently large

$$y_1 = y_0 + h\sum_{i=1}^{k} b_i J\nabla H(Y_i) \Longleftrightarrow y_1 = y_0 + h\int_0^1 J\nabla H((1-c)y_n + cy_1)dc$$

$\downarrow$ E.P. RK of order 2 $\qquad\qquad$ $\downarrow$ Averaged Vector Field Method

• G.R.W. Quispel, D.I. McLaren. A new class of energy-preserving numerical integration methods. *J. Phys. A* **41** (2008) 04526, 7.

• E. Celledoni, R.I. McLachlan, D. McLaren, B. Owren, G.R.W. Quispel, W.M. Wright. Energy preserving Runge-Kutta methods. M2AN **43** (2009) 645–649.

EQUIVALENT METHODS: Let $\nu = \deg(H(y)$. All the methods that realize the above equivalency are "*e*quivalent", namely they provide the very same numerical solution.

EXAMPLE: The trapezoidal method and the implicit midpoint method are equivalent if applied to linear autonomous Hamiltonian systems.

HOW CAN THE PREVIOUS APPROACH BE GENERALIZED IN ORDER TO GET HIGHER ORDER ENERGY-PRESERVING RUNGE-KUTTA METHODS?

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

[2009] - F.I., D. Trigiante. High-order symmetric schemes for the energy conservation of polynomial Hamiltonian problems. *J. Numer. Anal. Ind. Appl. Math.* **4**,1-2 (2009) 87–111.

[2009] - L. Brugnano, F.,I., D. Trigiante. Analysis of Hamiltonian Boundary Value Methods (HBVMs) for the numerical solution of polynomial Hamiltonian dynamical systems. 2009, *Submitted*, (`arXiv:0909.5659`).

The ingredients

1. A set of abscissae $0 \leq c_1 < \cdots < c_k \leq 1$ and weights $b_1, \ldots, b_k$ yielding a quadrature formula of suitable degree of precision d.

2. A polynomial $\sigma(t)$ of degree $s \leq k$, with $\sigma(t_0) = y_0$, defined for $t \in [t_0, t_0 + h]$ by means of the expansion

$$\dot{\sigma}(t_0+ch) = \sum_{j=1}^{s} \gamma_j P_j(c) \Longrightarrow Y_i \equiv \sigma(t_0+c_i h) = y_0+h\sum_{j=1}^{s} \gamma_j \int_0^{c_i} P_j(x)\,\mathrm{d}x,$$

   where $P_j(c)$ is the Legendre polynomial of degree $j-1$ shifted on $[0,1]$, and the (vector) coefficients $\{\gamma_j\}$ are to be regarded as unknown.

3. $y_1 = \sigma(t_0 + h)$ will yield the approximation to $y(t_0 + h)$.

High order Energy Preserving R-K methods

$$
\begin{aligned}
H(y_1) - H(y_0) &= \int_{t_0}^{t_0+h} (\dot\sigma(t))^T \nabla H(\sigma(t)) \mathrm{d}t \\
&= h \sum_{j=1}^{s} \gamma_j^T \int_0^1 P_j(c) \nabla H(\sigma(t_0 + ch)) \mathrm{d}c
\end{aligned}
$$

which vanishes by choosing, for $j = 1, \ldots, s$,

$$
\gamma_j = \eta_j \underbrace{\int_0^1 P_j(\tau) J \nabla H(\sigma(t_0 + ch)) \mathrm{d}c}_{\text{polynomial of degree} \le \nu s - 1} = \eta_j \underbrace{\sum_{\ell=1}^{k} b_\ell P_j(c_\ell) J \nabla H(\sigma(t_0 + c_\ell h))}_{\text{provided } d \ge \nu s - 1}.
$$

- η_j are suitable nonzero scaling factors that make the resulting method consistent

$$
\eta_j = \left(\int_0^1 P_j^2(x) \mathrm{d}x \right)^{-1}, \qquad j = 1, \ldots, s
$$

WE CAN FOLLOW TWO ROUTES

RUNGE-KUTTA FORMULATION

BLOCK-BVM FORMULATION

- Each formulation brings some advantages.
- Block-BVMs are a subclass of R-K methods;

RUNGE-KUTTA FORMULATION 1/2

$$Y_i = y_0 + h \sum_{j=1}^{s} \eta_j \int_0^{c_i} P_j(x)\mathrm{d}x \sum_{\ell=1}^{k} b_\ell P_j(c_\ell)\, f(Y_\ell).$$

Define the matrices $\mathcal{I}, \mathcal{P} \in \mathbb{R}^{k\times s}$ and Λ, Ω as

$$\mathcal{I}_{ij} = \int_0^{c_i} P_j(x)\mathrm{d}x, \quad \mathcal{P}_{ij} = P_j(c_i), \quad \begin{array}{l} \Lambda = \mathrm{diag}(\eta_1, \ldots, \eta_s), \\ \Omega = \mathrm{diag}(b_1, \ldots, b_k) \end{array}$$

We get the R-K method defined by the tableau

$$\begin{array}{c|c} c_1 & \\ \vdots & \mathcal{I}\Lambda\mathcal{P}^T\Omega \\ c_k & \\ \hline & b_1 \ \ldots \ b_k \end{array} \qquad (*)$$

THEOREM

Assume that

- $P_j(c)$, $j = 1, \dots, s$, is the shifted Legendre polynomial of degree $j-1$, on the interval $[0,1]$;
- the quadrature formula with abscissae $c_1 < \cdots < c_k$ and weights $b_1, \dots, b_k$ has degree of precision $d \geq 2s-1$.

Then the R-K method (*)

1. has order $2s$ for all $k \geq s$;
2. is symmetric and precisely A-stable;
3. becomes the Gauss-Legendre method of order $2s$, when $k = s$;
4. is energy preserving when applied to canonical polynomial Hamiltonian systems with Hamiltonian function $H(y)$ of degree $\nu \leq \frac{d+1}{s}$ (if the c_i are the Gauss abscissae then $\nu \leq \frac{2k}{s}$).

LINK TO COLLOCATION METHODS 1/2

Consider a collocation method with k stages, defined by the tableau

$$\begin{array}{c|c} c_1 & \\ \vdots & \mathcal{A} \\ c_k & \\ \hline & b_1 \ \ldots \ b_k \end{array} \qquad \mathcal{A} = (\alpha_{ij}) \equiv \left(\int_0^{c_i} \ell_j(x)\mathrm{d}x \right), \qquad b_j = \int_0^1 \ell_j(x)\mathrm{d}x,$$

$\ell_j(c)$ being the jth Lagrange polynomial of degree $k-1$ defined on the set of abscissae $\{c_i\}$. Assume that the quadrature formula (c_i, b_i) has degree of prec. $\geq 2s-1$. Let

- $\Omega = \mathrm{diag}(b_1, \ldots, b_k)$,
- $\widehat{P}_j(t)$, $j = 1, \ldots, s$, the normalized shifted Legendre polynomial of degree $j-1$, on the interval $[0, 1]$,
- $\mathcal{P}_s = (\widehat{P}_j(c_i))$ ($k \times s$ matrix)

LINK TO COLLOCATION METHODS 2/2 ([2010])

The Energy Preserving R-K method (*) may be recast as

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

[2010] - L.Brugnano, F.I., D.Trigiante. The Lack of Continuity and the Role of Infinite and Infnitesimal in Numerical Methods for ODEs: the Case of Symplecticity, Applied Mathematics and Computation, (to appear) (arXiv:1010.4538).

REMARK: Note that the Butcher array A has rank which cannot exceed s, because it is defined by *filtering* the Butcher array $\mathcal{A}$ associated with a standard collocation method by the rank s matrix $\mathcal{P}_s \mathcal{P}_s^T \Omega$. As a consequence, $k - s$ of the internal stages, that we called *silent stages*, may be cast as linear combinations of the remaining s *fundamental stages* and the nonlinear system to be solved at each step of the integration procedure has actually block-dimension s rather than k. This is better visualized by recasting the method in block-BVM form (next slide).

ALTERNATIVE FORMULATION

The first approach used to devise the new methods has led to their formulation in terms of block-Boundary Value Methods rather than Runge-Kutta methods. Consequently, they have been named Hamiltonian Boundary Value Methods: HBVM(k,s).
The nonlinear system takes the form

$$\begin{pmatrix} -e & I_s & 0_{s\times r} \\ -a_0 & -A_1 & I_r \end{pmatrix} \otimes I_{2m}\,\widehat{Y} = h \begin{pmatrix} b_0 & B_1 & B_2 \\ \mathbf{0} & 0_{r\times s} & 0_{r\times r} \end{pmatrix} \otimes J\,\nabla H(\widehat{Y}).$$

where

$$\widehat{Y} = \begin{cases} [Y_1^T, \dots, Y_k^T]^T, & \text{if } Y_1 = y_0, \\ [Y_1^T, \dots, Y_k^T]^T, & \text{if } Y_1 = y_0, \end{cases}$$

REMARK: The HBVM formulation is more appropriate for implementation, since it uncouples the linear and nonlinear part of the system.

Infinity HBVMs

These are the limit as $k \to \infty$ of HBVM(k,s)

$$\text{HBVM}(\infty, s) = \lim_{k\to\infty} \text{HBVM}(k, s).$$

This is tantamount to retain the integrals in place of the quadrature formulae:

$$Y_i = y_0 + h\int_0^1 \left(\sum_{j=1}^{s} \eta_j a_{ij} P_j(\tau)\right) J\nabla H(\sigma(t_0+\tau h))\mathrm{d}\tau, \qquad i = 1, \ldots, s.$$

The limit formula with $\{P_j\}$ the Lagrange basis was first devised by E. Hairer.

[2010] - E. Hairer, Energy-preserving variant of collocation methods, *J. Numer. Anal. Ind. Appl. Math.*, **5**,1-2 (2010).

[2010] - L. Brugnano, F.I., D. Trigiante, Hamiltonian Boundary Value Methods (Energy Preserving Discrete Line Integral Methods). *Jour. of Numer. Anal., Industr. and Appl. Math.* **5**,1-2 (2010) 17–37. (`arXiv:0910.3621`)

Local Fourier expansion of the problem 1/2 [2010]

$$y'(t) = f(y(t)), \qquad t \in [t_0, t_0 + h], \qquad y(t_0) = y_0 \in \mathbb{R}^m,$$

Let us consider an orthonormal basis $\{P_j\}_{j\geq 1}$, for example the Legendre polynomials on the interval [0,1]:

$$\int_0^1 P_i(\tau)P_j(\tau)\mathrm{d}\tau = \delta_{ij}, \qquad \deg(P_j) = j - 1.$$

By expanding the right-hand side of the equation, we obtain:

$$y'(t_0 + ch) = \sum_{j=1}^{\infty} \gamma_j(y; h)P_j(c), \qquad c \in [0, 1],$$

with the Fourier coefficients given by

$$\gamma_j(y; h) = \int_0^1 P_j(\tau)f(y(t_0 + \tau h))\mathrm{d}\tau.$$

Local Fourier expansion of the problem 2/2

By truncating the expansion after k terms, we obtain the problem

$$\sigma'(t_0 + ch) = \sum_{j=1}^{k} \gamma_j(\sigma; h) P_j(c), \qquad c \in [0, 1],$$

with

$$\gamma_j(\sigma; h) = \int_0^1 P_j(\tau) f(\sigma(t_0 + \tau h)) \mathrm{d}\tau.$$

Its solution, formally given by

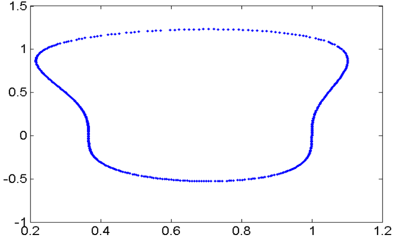
$$\sigma(t_0 + ch) = y_0 + h \sum_{j=0}^{r-1} \gamma_j(\sigma; h) \int_0^c P_j(\tau) \mathrm{d}\tau, \qquad c \in [0, 1],$$

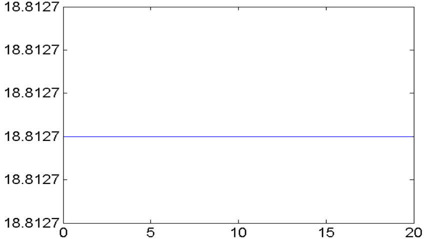
is a polynomial of degree r.

POLYNOMIAL EXAMPLE

$$H(p,q) = \frac{1}{3}p^3 - \frac{1}{2}p + \frac{1}{30}q^6 + \frac{1}{4}q^4 - \frac{1}{3}q^3 + \frac{1}{6}.$$

E. Faou, E. Hairer and T.-L. Pham, *Energy conservation with non-symplectic methods: Examples and counter-examples*, BIT 44, no. 4 (2004)





- HBVM of order 4 and degree of precision 6, $h = 1$, $(q_0, p_0) = (0, 1)$.
- LEFT Picture: (p, q)-plane.
- RIGHT Picture: Energy function $H(y_n)$

NON-POLYNOMIAL EXAMPLE 1/3

The Hamitonian function

$$H(x,y,z,\dot{x},\dot{y},\dot{z}) = \frac{1}{2m}\left[\left(\dot{x}-\alpha\frac{x}{\varrho^2}\right)^2+\left(\dot{y}-\alpha\frac{y}{\varrho^2}\right)^2+(\dot{z}+\alpha\log(\varrho))^2\right]$$

with $\varrho=\sqrt{x^2+y^2}$, $\alpha = e\,B_0$, m is the particle mass, e is its charge, and B_0 is the magnetic field intensity, defines the motion of a charged particle in a magnetic field under Biot-Savart potential.

We have integrated with the values

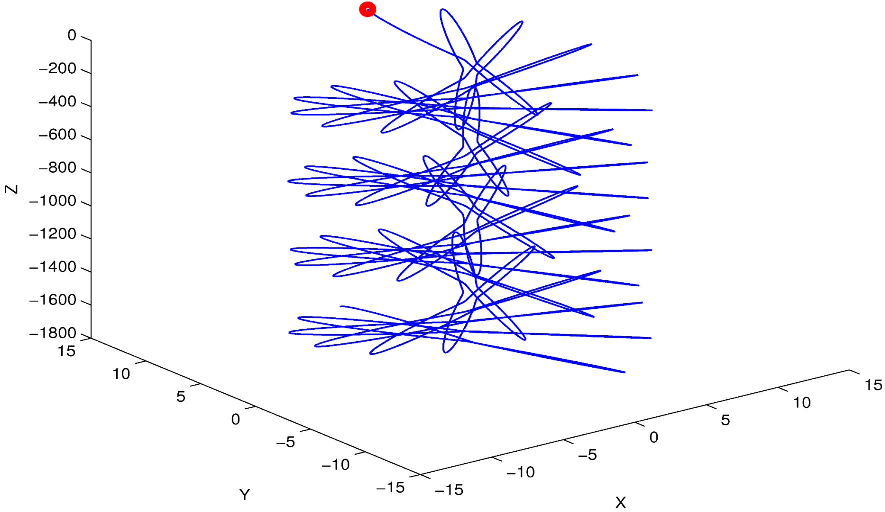
$$m=1, \qquad e=-1, \qquad B_0=1,$$

with starting point

$$x=0.5, \quad y=10, \quad z=0, \quad \dot{x}=-0.1, \quad \dot{y}=-0.3, \quad \dot{z}=0.$$

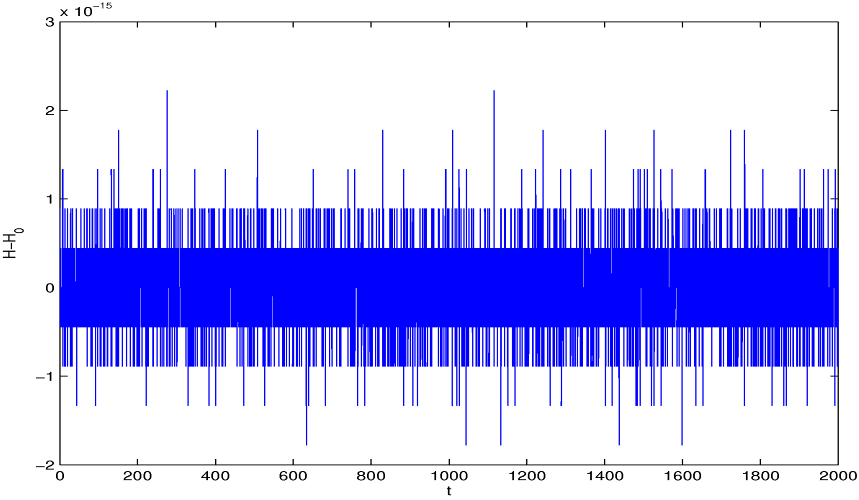
NON-POLYNOMIAL EXAMPLE 2/3

Solution curve in the 3D space.



NON-POLYNOMIAL EXAMPLE 3/3

Error in the energy function $H(y_n) - H(y_0)$ associated with HBVM(6,2) (order 4, exact for $\deg(H) \le 6$ (Gaussian distribution).)



KEPLER PROBLEM WITH NON-CONSTANT STEPSIZE

Hamiltonian:

$$H(q,p) = \frac{1}{2}\left(p_1^2 + p_2^2\right) - \frac{1}{\sqrt{q_1^2 + q_2^2}}.$$

Initial condition:

$$q_1 = 1 - e, \qquad q_2 = 0, \qquad p_1 = 0, \qquad p_2 = \sqrt{(1+e)/(1-e)}.$$

Periodic elliptic orbit:

with eccentricity e and period 2π.

Costant stepsize is not efficient, when the eccentricity is close to 1:

a variable mesh selection would be more appropriate.

Standard mesh selection

Let p be the order of the method, then:

$$h_{new} = 0.7 \cdot h_n \left(\frac{Tol}{err_n} \right)^{1/(p+1)},$$

where err_n is a suitable estimate of the local error.

Kepler problem, $e = 0.99$

Sixth order methods:

- GAUSS6: 3-stages Gauss-Legendre method (symplectic);
- HBVM(12,3): practically energy-conserving, in such a case.

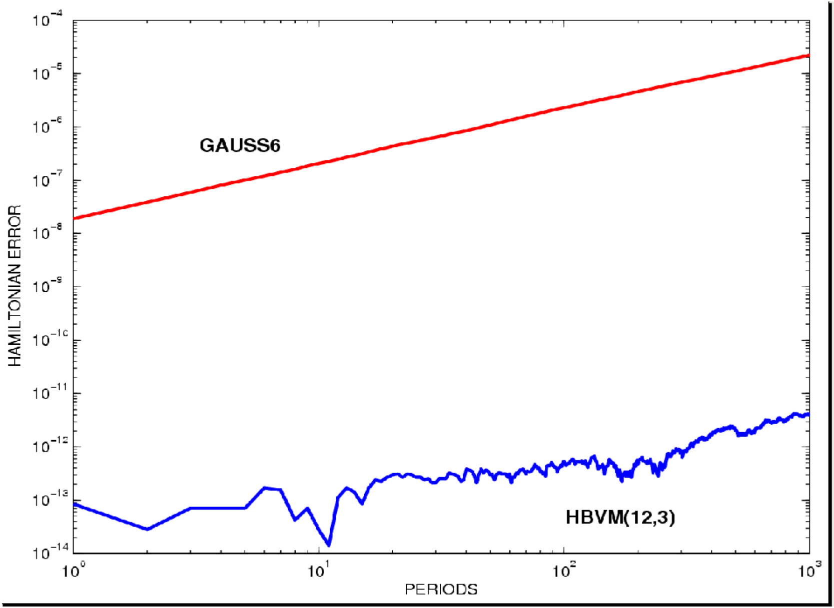
Time interval:

1000 periods.

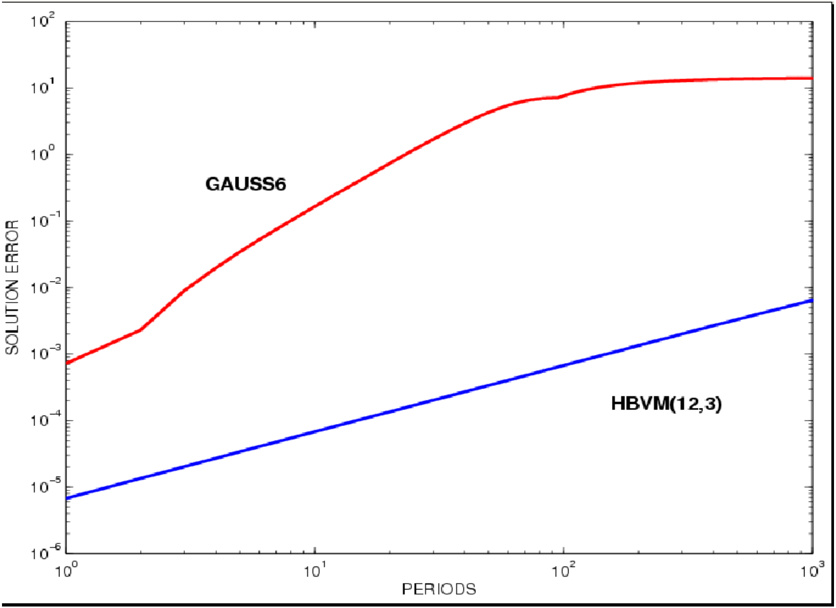
Tolerance:

10^{-10}.

Hamiltonian error



Solution error



What is the gain? By using the tollerance $Tol = 10^{-10}$,

the variable stepsize implementation

of HBVM(12,3) requires 153 steps per period.

To obtain the same accuracy,

the constant stepsize implementation

of GAUSS6 would require $\approx 2 \cdot 10^5$ steps per period!

http://www.math.unifi.it/~brugnano/HBVM/

Hamiltonian Boundary Value Methods (HBVMs)

Energy Preserving Discrete Line Integral Methods

Hamiltonian BVMs (HBVMs) constitute a class of energy-preserving methods for the numerical solution of canonical Hamiltonian systems, i.e., problems in the form:

$$\dot{y} = J\nabla H(y), \qquad y(t_0) = y_0 \in \mathbb{R}^{2m},$$

where J is a constant skew-symmetric matrix, and $H(y)$ is the Hamiltonian function. Such methods are able to preserve, in the numerical solution, the value of the Hamiltonian function, as it happens for the continuous one. Hereafter, are the main facts about HBVMs:

1. Basic Facts about HBVMs
2. Some Numerical Tests
3. Infinity HBVMs
4. Isospectral Property of HBVMs and their connections with RK collocation methods
5. Blended HBVMs
6. Notes and References (downloadable)
7. Matlab Codes (new)
8. HBVMs Test Gallery
9. Contacts
10. Recent developments (updated September 7, 2010)