Rendiconti Sem. Mat. Univ. Pol. Torino
Vol. 76, 2 (2018), 123 – 134

F. Iavernaro [*] - F. Mazzia[†]

ON CONJUGATE-SYMPLECTICITY PROPERTIES OF A MULTI-DERIVATIVE EXTENSION OF THE MIDPOINT AND TRAPEZOIDAL METHODS[‡]

Abstract. Conjugate symplecticity up to order $p+2$ of p-th one-step multi-derivative methods based on an extension of the midpoint and trapezoidal methods is proved. If compared with similar achievements obtained for the class of Euler-MacLauren and Hermite-Obreshkov methods, this result further confirm that multi-derivative methods, despite failing in achieving the symplecticity property, may play a significant role in the context of geometric integration. A numerical illustration has also been added.

1. Introduction

The present work focuses on the symplecticity properties of two families of multi-derivative high-order one-step methods which contain the well-known implicit midpoint and trapezoidal methods as seed formulae. In more detail, we consider the applications of such multi-derivative integrators to canonical Hamiltonian problems

$$y' = J\nabla H(y), \qquad y(t_0) = y_0 \in \mathbb{R}^{2m}, \tag{1.1}$$

with

$$y = \begin{pmatrix} q \\ p \end{pmatrix}, \quad q, p \in \mathbb{R}^m, \qquad J = \begin{pmatrix} O & I \\ -I & O \end{pmatrix}, \tag{1.2}$$

where q and p stand for the generalized coordinates and conjugate momenta respectively, while $H : \mathbb{R}^{2m} \to \mathbb{R}$ is the Hamiltonian function and I is the identity matrix of dimension m.

As is well-known, symplecticity is a characterizing property of canonical Hamiltonian systems such as (1.1) and means that the associated flow $\varphi_t : y_0 \to y(t)$ has Jacobian matrix satisfying

$$\frac{\partial \varphi_t(y)^\top}{\partial y} J \frac{\partial \varphi_t(y)}{\partial y} = J, \quad \text{for all } y \in \mathbb{R}^{2m}. \tag{1.3}$$

Likewise, a one-step method $y_1 = \Phi_h(y_0)$ (h is the stepsize of integration) is called symplectic if its Jacobian matrix is symplectic, i.e. Φ_h satisfies the analog of (1.3) with $\Phi_h(y)$ in place of $\varphi_t(y)$.

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[*] Dipartimento di Matematica, Università degli studi di Bari Aldo Moro.

[†] Dipartimento di Informatica, Università degli studi di Bari Aldo Moro.

[‡] This work was funded by the INdAM-GNCS 2018 Research Project "Numerical methods in optimization and ODEs" (the authors are members of the INdAM Research group GNCS)

In the context of geometric integration, the study of symplecticity, as a property inherited by a numerical scheme, plays a prominent role since it significantly influences the qualitative behavior of the numerical solutions in many respects. As a matter of fact, a symplectic integrator displays interesting features such as volume preservation of closed surfaces in the phase space under time evolution, conservation of all quadratic first integrals and near conservation of the Hamiltonian function over exponentially long times [5, page 366].

Unfortunately, the multi-derivative approach addressed to extend the class of irreducible Runge–Kutta methods was shown to be incompatible with the symplecticity property [7]. This negative result partly eclipsed a further theoretical investigation of multi-derivative methods, although numerical evidence of their good long-time behavior has been highlighted in several numerical experiments (see, for example, [12]).

The non-existence of multi-derivative R–K methods does not preclude the possibility for these methods to share some weaker geometric properties. A one-step method $y_1 = \Phi_h(y_0)$ is conjugate-symplectic if it is topologically conjugate to a symplectic method $y_1 = \Psi_h(y_0)$. This means that a global change of coordinates $\chi_h(y) = y + O(h)$ exists such that $\Phi_h = \chi_h \circ \Psi_h \circ \chi_h^{-1}$. The solution $\{y_n\}$ of a symplectic conjugate method thus satisfies

$$y_n = \Phi_h^n(y_0) = (\chi_h \circ \Psi_h \circ \chi_h^{-1})^n(y_0) = \chi_h \circ \Psi_h^n \circ \chi_h^{-1}(y_0)$$

which implies that the trajectories in the phase space generated by a conjugate symplectic method inherit the same qualitative behaviour as those produced by a symplectic method. A more relaxed property, shared by a wider class of numerical schemes, is a generalization of the conjugate-symplecticity property, introduced in [8]. A method $y_1 = \Phi_h(y_0)$ of order p is conjugate-symplectic up to order $p+r$, with $r \geqslant 0$, if a global change of coordinates $\chi_h(y) = y + O(h^p)$ exists such that $\Phi_h = \chi_h \circ \Psi_h \circ \chi_h^{-1}$, with the map Ψ_h satisfying

$$\Psi_h'(y)^T J \Psi_h'(y) = J + O(h^{p+r+1}). \tag{1.4}$$

A consequence of property (1.4) is that the method $\Phi_h(y)$ nearly conserves all quadratic first integrals and the Hamiltonian function over time intervals of length $O(h^{-r})$ (see [8]).

The question whether conjugate-symplectic up to order $p+r$ multi-derivative methods might exist has been recently addressed. In [9] the authors proved that the family of Euler–MacLaurin formulae are conjugate-symplectic up to order $p+2$. A further instance of conjugate-symplectic up to order $p+2$ multi-derivative methods appears in [11], and is based on a special subclass of Hermite–Obrechkoff methods which admit a continuous spline extension. The present study is a further step on this path of investigation. Though not considered here, it is worth mentioning that this recent interest in studying multi-derivative geometric integrators is partly motivated by the availability of a new tool to efficiently compute the higher derivatives of the vector field needed during the implementation of the methods, namely the Infinity Computer. This is a new type of a computing architecture allowing one to work *numerically* with infinite and infinitesimal numbers (see [1, 10, 13, 14, 15] and reference therein).

The paper is organized as follows: in Section 2, we formally derive the extensions of the implicit midpoint and trapezoidal methods we are interested in. In Section 2, we show the conjugate symplecticity properties of such integrators. Finally, Section 3 contains a numerical illustration.

2. Derivation of the method

The multi-derivative generalization of the midpoint (MP) and trapezoidal (TR) method we are interested in is easily obtained via a standard Taylor approach by exploiting the property that such classical schemes may be viewed as composition of the Implicit (IE) and Explicit Euler (EE) methods, in direct and reverse order, applied on half the integration time-step:

$$\text{MP} = \text{EE} \circ \text{IE}: \quad y_1 = y_0 + hf(\frac{y_0+y_1}{2}) \qquad \Longleftrightarrow \qquad \begin{cases} y_{1/2} = y_0 + \frac{h}{2} f(y_{1/2}), \\ y_1 = y_{1/2} + \frac{h}{2} f(y_{1/2}), \end{cases}$$

$$\text{TR} = \text{IE} \circ \text{EE}: \quad y_1 = y_0 + \frac{h}{2}(f(y_0)+f(y_1)) \qquad \Longleftrightarrow \qquad \begin{cases} y_{1/2} = y_0 + \frac{h}{2} f(y_0), \\ y_1 = y_{1/2} + \frac{h}{2} f(y_1). \end{cases}$$

Given the initial value problem defined on the time window $[0,h]$

$$y'(ch) = f(y(ch)), \quad c \in [0,1], \quad y(0) = y_0,$$

and exploiting its integral form

$$y(ch) = y_0 + h\int_0^c f(y(\tau h))\mathrm{d}\tau,$$

we get

$$\begin{cases} y(h/2) = y_0 + h\displaystyle\int_0^{1/2} f(y(\tau h))\mathrm{d}\tau, \\ y(h) = y(h/2) + h\displaystyle\int_{1/2}^{1} f(y(\tau h))\mathrm{d}\tau. \end{cases} \tag{2.5}$$

In order to obtain high-order numerical schemes, we approximate the two integrand functions by means of their Taylor expansion around one of the two endpoints up to a given order. More precisely, mimiking the composition procedure discussed above for the TR and MP formulae, we follow two different approaches.

2.1. Multi-derivative midpoint (MDMP) method

We consider the expansion of $f(y(\tau h))$ in a neighbourhood of $\tau = 1/2$:

$$f(y(\tau h)) = \sum_{i=0}^{R} \frac{h^i}{i!} y^{(i+1)}(h/2)\left(\tau - \frac{1}{2}\right)^i + O(h^{R+1}), \tag{2.6}$$

where $y^{(i+1)}(t) = D^i f(y(t))$. Observing that

$$\int_0^{1/2}\left(\tau-\frac{1}{2}\right)^i \mathrm{d}\tau = \frac{(-1)^i}{i+1}\left(\frac{1}{2}\right)^{i+1}, \qquad \int_{1/2}^{1}\left(\tau-\frac{1}{2}\right)^i \mathrm{d}\tau = \frac{1}{i+1}\left(\frac{1}{2}\right)^{i+1},$$

we plug (2.6) into (2.5) after neglecting the infinitesimal term $O(h^{R+1})$. In so doing, we obtain the one-step multi-derivative composition method

$$\left\{\begin{aligned} y_{1/2} &= y_0 + \frac{h}{2}f(y_{1/2}) + \sum_{i=1}^{R}(-1)^i\left(\frac{h}{2}\right)^{i+1}\frac{D_i f(y_{1/2})}{(i+1)!},\\ y_1 &= y_{1/2} + \frac{h}{2}f(y_{1/2}) + \sum_{i=1}^{R}\left(\frac{h}{2}\right)^{i+1}\frac{D_i f(y_{1/2})}{(i+1)!}, \end{aligned}\right. \tag{2.7}$$

where, for any given vector z, $D_i f(z)$ denotes the total i-th time derivative of $f(y(t))$ evaluated at $y(t) = z$:

$$D_i f(z) = \left.\frac{\mathrm{d}^i}{\mathrm{d}t^i} f(y(t))\right|_{y(t)=z}.$$

We use the subscript D_i to distinguish the operator from the classical time-derivative operator of order i which will be denoted, as usual, by D^i. One solves the first (in general nonlinear) equation in the unknown $y_{1/2}$ and then computes the approximation y_1 by means of the second explicit formula. Summing both sides of the two equations yields

$$y_1 = y_0 + hf(y_{1/2}) + 2\sum_{\substack{i=2\\ i\,\text{even}}}^{R}\left(\frac{h}{2}\right)^{i+1}\frac{D^i f(y_{1/2})}{(i+1)!}. \tag{2.8}$$

We see that, the choices $R = 0, 1$, lead back to the MP formula while, for $R \geqslant 2$ the local truncation error is $O(h^{R+3})$ when R is even, and $O(h^{R+2})$ when R is odd. Consequently, the order of convergence of (2.8) is $p = R+2$ for even values of R, and $p = R+1$ for odd values of R. Since the former case is more favourable, we will make the choice $R = 2s$ in the following.

2.2. Multi-derivative trapezoidal (MDTR) method

Reversing the order of composition of the two methods in (2.7) is tantamount to use the Taylor polynomials of $f(y(\tau h))$ expanded at 0 and 1 inside the two integrals appearing in (2.5), respectively. This procedure gives rise to the one-step multi-derivative composition method

$$
\left\{
\begin{aligned}
y_{1/2} &= y_0 + \frac{h}{2} f(y_0) + \sum_{i=1}^{R} \left(\frac{h}{2}\right)^{i+1} \frac{D_i f(y_0)}{(i+1)!}, \\
y_1 &= y_{1/2} + \frac{h}{2} f(y_1) + \sum_{i=1}^{R} (-1)^i \left(\frac{h}{2}\right)^{i+1} \frac{D_i f(y_1)}{(i+1)!}.
\end{aligned}
\right. \tag{2.9}
$$

Again, for $R = 0$ we get the TR method while, for $R \geqslant 1$ the resulting order of convergence is $p = R+2$ or $p = R+1$ according to the parity of R as illustrated above for the MDMP method. Summing both sides of the two equations yields

(2.10)

$$
y_1 = y_0 + \frac{h}{2}(f(y_0) + f(y(1))) + \sum_{i=1}^{R} \left(\frac{h}{2}\right)^{i+1} \frac{1}{(i+1)!} \left(D_i f(y_0) + (-1)^i D_i f(y_1)\right).
$$

which is a one-step scheme in the class of Hermite-Obrechkov methods.

3. Conjugate Symplecticity Properties.

In this section we prove that MDMP and MDTR methods are conjugate symplectic integrators up to order $p+2 = 2s+4$. The two families of schemes are evidently topologically conjugate since, by definition, these methods are obtained by composing two one-step methods in direct and reverse order (compare (2.7) with (2.9)). Therefore, hereafter we address our investigation to MDTR methods which are more easily handled.

To prove that the MDTR formula is conjugate to a symplectic method up to order $p+2 = 2s+4$, we show that the map $y_1 = \Psi_h(y_0)$ associated with the MDTR method is such that $\Psi_h(y) = \Phi_h(y) + O(h^{2s+5})$, where $y_1 = \Phi_h(y_0)$ is a suitable B-series integrator satisfying property (a) of the following lemma taken from [3] . We recall that a numerical method can be expressed as a formal B-series if it admits a power series expansion in the time step where each term is a sum of elementary differentials of the vector field (see [6] for details).

LEMMA 1. *[3] Assume that problem (1.1) admits a quadratic first integral* $Q(\mathbf{y}) = \mathbf{y}^T S \mathbf{y}$, *where* S *denotes a constant symmetric matrix, and is solved by a B-series integrator* $\Phi_h(\mathbf{y})$. *Then, the following properties are equivalent:*

- *(a)* $\Phi_h(\mathbf{y})$ *admits a modified first integral expanded as a formal series in the form* $\widetilde{Q}(\mathbf{y}) = Q(\mathbf{y}) + hQ_1(\mathbf{y}) + h^2 Q_2(\mathbf{y}) + \ldots$, *where each* $Q_i(\cdot)$ *is a differential functional;*
- *(b)* $\Phi_h(\mathbf{y})$ *is conjugate to a symplectic B-series integrator.*

We will follow the very same lines of the proof given in [9], where the geometric properties of the Euler-Maclaurin multi-derivative one-step methods have been investigated.

THEOREM 1. *The map* $y_1 = \psi_h(y_0)$ *associated with the one-step multi-derivative method (2.10) admits a B-series expansion and is conjugate to a symplectic B-series integrator up to order* $2s+4$.

Proof. The existence of a B-series expansion for $y_1 = \Psi_h(y_0)$ is directly deduced from [7], where a B-series representation of a generic multi-derivative Runge-Kutta method has been obtained.

Given a stepsize h, we look for an analytic function $v(t)$ formally satisfying the difference equation (2.10), where we set $R = 2s$. Denoting by E_h the shift operator, namely $E_h(v(t)) = v(t+h)$, we get

$$\begin{aligned} v(t+h) =& v(t) + \frac{h}{2}(f(v(t)) + f(v(t+h))) + \\ &+ \sum_{i=1}^{2s} \left(\frac{h}{2}\right)^{i+1} \frac{1}{(i+1)!} \big(D_i f(v(t)) + (-1)^{i+1} D_i f(v(t+h))\big)\,. \end{aligned}$$

After organizing the sums in odd and even indices, we obtain

$$\begin{aligned} v(t+h) =& v(t) + \frac{h}{2}(f(v(t)) + f(v(t+h))) \\ &+ \sum_{i=1}^{s} \left(\frac{h}{2}\right)^{2i} \frac{1}{(2i)!} D_{2i-1}(f(v(t)) - f(v(t+h))) \\ &+ \sum_{i=1}^{s} \left(\frac{h}{2}\right)^{2i+1} \frac{1}{(2i+1)!} D_{2i}(f(v(t)) + f(v(t+h)). \end{aligned}$$

In terms of the two characteristic polynomials defining the classical trapezoidal method,

$$\rho(z) := z - 1, \qquad \sigma(z) := \frac{1}{2}(z+1),$$

the latter equation reads

$$\begin{aligned} \rho(E_h)v(t) =& h\sigma(E_h) f(v(t)) + \sum_{i=1}^{s} \left(\frac{h}{2}\right)^{2i+1} \frac{2}{(2i+1)!} \sigma(E_h) D_{2i} f(v(t)) \\ &- \sum_{i=1}^{s} \left(\frac{h}{2}\right)^{2i} \frac{1}{(2i)!} \rho(E_h) D_{2i-1} f(v(t)). \end{aligned}$$

Recalling the relationship between the shift and derivative operators,

$$E_h = \sum_{j=0}^{\infty} \frac{h^j}{j!} D^j \equiv e^{hD},$$

we obtain

$$\begin{aligned}\rho(e^{hD})v(t) =& h\sigma(e^{hD})f(v(t))+\sum_{i=1}^{s}\left(\frac{h}{2}\right)^{2i+1}\frac{2}{(2i+1)!}\sigma(e^{hD})D_{2i}f(v(t))\\ &-\sum_{i=1}^{s}\left(\frac{h}{2}\right)^{2i}\frac{1}{(2i)!}\rho(e^{hD})D_{2i-1}f(v(t)).\end{aligned}$$

Multiplying both sides of the previous equation by $D\rho(e^{hD})^{-1}$ yields

$$\begin{aligned}Dv(t) =& hD\rho(e^{hD})^{-1}\sigma(e^{hD})f(v(t))+\sum_{i=1}^{s}\left(\frac{h}{2}\right)^{2i}\frac{hD}{(2i+1)!}\rho(e^{hD})^{-1}\sigma(e^{hD})D_{2i}f(v(t))\\ &-\sum_{i=1}^{s}\left(\frac{h}{2}\right)^{2i}\frac{DD_{2i-1}}{(2i)!}f(v(t)),\end{aligned}$$

that is,

$$\begin{aligned}\dot{v}(t) =& hD\rho(e^{hD})^{-1}\sigma(e^{hD})\left(I+\sum_{i=1}^{s}\left(\frac{h}{2}\right)^{2i}\frac{D_{2i}}{(2i+1)!}\right)f(v(t))\\ &-\sum_{i=1}^{s}\left(\frac{h}{2}\right)^{2i}\frac{DD_{2i-1}}{(2i)!}f(v(t)).\end{aligned}$$

We now exploit the generating function of Bernoulli numbers

$$\frac{z}{e^z-1}=\sum_{k=0}^{\infty}B_k\frac{z^k}{k!},$$

where $B_0=1, B_1=-1/2$ and $B_j=0$ for the other odd j, to see that

$$\frac{z\sigma(e^z)}{\rho(e^z)}=\frac{1}{2}\frac{z(e^z+1)}{e^z-1}=\frac{z}{e^z-1}+\frac{z}{2}=1+\sum_{j=1}^{\infty}\frac{B_{2j}}{(2j)!}z^{2j}.$$

Thus, we arrive at

$$\begin{aligned}\dot{v}(t)=&\Bigg(\left(I+\sum_{j=1}^{\infty}\frac{B_{2j}}{(2j)!}h^{2j}D^{2j}\right)\left(I+\sum_{i=1}^{s}\left(\frac{h}{2}\right)^{2i}\frac{D_{2i}}{(2i+1)!}\right)\\ &-\sum_{i=1}^{s}\left(\frac{h}{2}\right)^{2i}\frac{DD_{2i-1}}{(2i)!}\Bigg)f(v(t)).\end{aligned}$$

Adding and subtracting terms involving the classical derivative operator D^{2i}, we get

$$\begin{aligned}\dot{v}(t) = \Bigg(& \Big(I+\sum_{j=1}^{\infty}\frac{B_{2j}}{(2j)!}h^{2j}D^{2j}\Big)\Big(I+\sum_{i=1}^{s}\left(\frac{h}{2}\right)^{2i}\frac{D^{2i}}{(2i+1)!}+\sum_{i=1}^{s}\left(\frac{h}{2}\right)^{2i}\frac{D_{2i}-D^{2i}}{(2i+1)!}\Big)\\ & -\sum_{i=1}^{s}\left(\frac{h}{2}\right)^{2i}\frac{D^{2i}}{(2i)!}-\sum_{i=1}^{s}\left(\frac{h}{2}\right)^{2i}\frac{D(D_{2i-1}-D^{2i-1})}{(2i)!}\Bigg)f(v(t)),\end{aligned}$$

that we recast as

(3.11)

$$\begin{aligned}\dot{v}(t) = & \Bigg(\Big(I+\sum_{j=1}^{\infty}\frac{B_{2j}}{(2j)!}h^{2j}D^{2j}\Big)\Big(I+\sum_{i=1}^{s}\left(\frac{h}{2}\right)^{2i}\frac{D^{2i}}{(2i+1)!}\Big)-\sum_{i=1}^{s}\left(\frac{h}{2}\right)^{2i}\frac{D^{2i}}{(2i)!}\Bigg)f(v(t))\\ & +\Bigg(\Big(I+\sum_{j=1}^{\infty}\frac{B_{2j}}{(2j)!}h^{2j}D^{2j}\Big)\Big(\sum_{i=1}^{s}\left(\frac{h}{2}\right)^{2i}\frac{D_{2i}-D^{2i}}{(2i+1)!}\Big)-\sum_{i=1}^{s}\left(\frac{h}{2}\right)^{2i}\frac{D(D_{2i-1}-D^{2i-1})}{(2i)!}\Bigg)f(v(t)).\end{aligned}$$

Since $v(t)=y(t)+O(h^{2s+2})$, we see that $(D^j-D_j)f(\nu(t))=O(h^{2s+2}), j=1,\dots,2s$ and hence the solution $v(t)$ of (3.11) is $O(h^{2s+4})$-close to the solution of the following initial value problem

$$\dot{w}(t)=f(w(t))+\sum_{j=s+1}^{\infty}\delta_j h^{2j}D^{2j}f(w(t)), \tag{3.12}$$

with

$$\delta_j:=\sum_{k=0}^{s}\frac{B_{2(j-k)}}{(2(j-k))!}\frac{1}{2^{2k}(2k+1)!},$$

that has been derived from (3.11) by neglecting the sums containing the derivatives $D_{2i}-D^{2i}, D_{2i-1}-D^{2i-1}$. Observe that $\delta_j=0$ for $j=1,\dots,s$, since the method is of order $2(s+1)$ (see [6], Theorem 3.1, page 340). We may interpret (3.12) as the modified equation of a one-step method $y_1=\Phi_h(y_0)$, where Φ_h is evidently the time-h flow associated with (3.12). Expanding the solution of (3.12) in Taylor series, we get

$$\begin{aligned}\Phi_h(y_0) \quad = \quad & y_1=v(t_0+h)=y_0+hf(y_0)+\sum_{j=s+1}^{\infty}\delta_j h^{2j+1}D^{2j}f(y_0)\\ & +\frac{h^2}{2!}f'(y_0)f(y_0)+\sum_{j=s+1}^{\infty}\delta_j h^{2j+2}D^{2j+1}f(y_0)+\dots.\end{aligned}$$

Collecting like powers of h gives rise to a formal power series expansion in the stepsize h, that is a B-series expansion.

Finally, the proof of property (a) in Lemma 1 follows the very same steps of the analogous proof in Theorem 1 of [9] and therefore we omit the details. The result follows, since $\Psi_h(y)=\Phi_h(y)+O(h^{2s+5})$. □

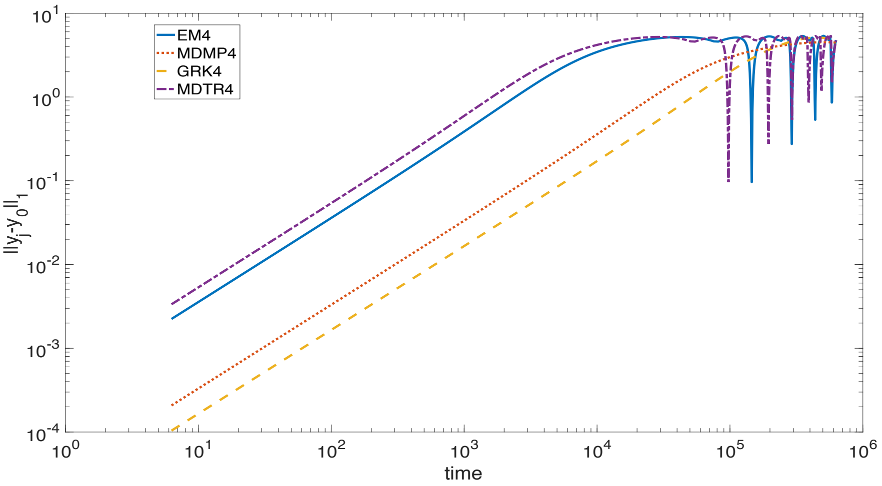

Figure 1: Kepler problem. Absolute error of the numerical solution for the order four methods: MDMP4 (red dotted line), MDTR4 (purple dashed-dotted line), EM4 (blue line), GRK4 (yellow dashed line).

4. A numerical illustration

We report an example to show the behavior of the order four MDMP and MDTR methods, and include comparisons with the Euler-Maclaurin method [9] and the symplectic Gauss R–K method of the same order. Throughout this section these methods will be labeled as MDMP4, MDTR4, EM4 and GRK4 respectively.

The test equation is the classical Kepler problem, which describes the motion of two bodies subject to Newton's law of gravitation. This problem is a completely integrable Hamiltonian nonlinear dynamical system with two degrees of freedom (see [2] for details). Its Hamiltonian function,

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

describes the motion of the body that is not located in the origin of the coordinate systems. This motion is an ellipse in the q_1-q_2 plane, whose eccentricity e is set using

$$q_1(0) = 1 - e, \quad q_2(0) = 0, \quad p_1(0) = 0, \quad p_2(0) = \sqrt{\frac{1+e}{1-e}}$$

as starting values. The corresponding period is $\mu := 2\pi$. Aside the total energy H, a further first integral of this problem is the angular momentum

$$M(q_1, q_2, p_1, p_2) := q_1 p_2 - q_2 p_1.$$

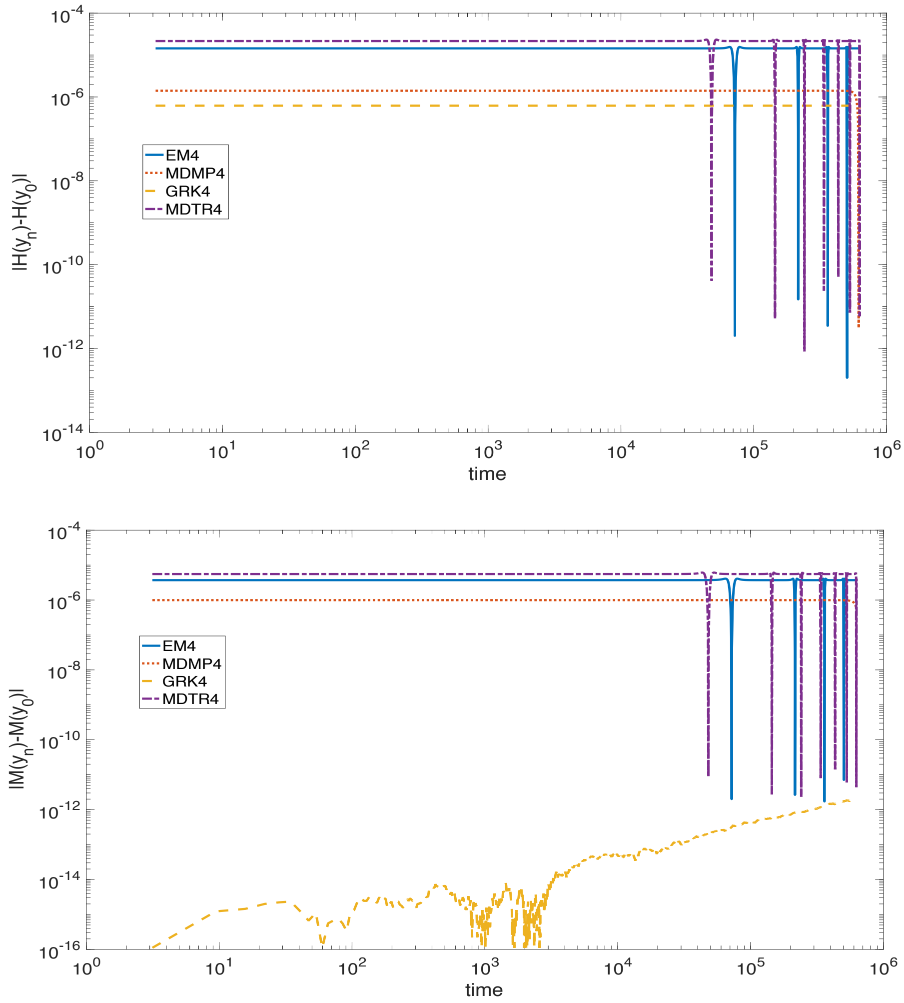

Figure 2: Kepler problem. Results for the order four methods: MDMP4 (red dotted line), MDTR4 (purple dashed-dotted line), EM4 (blue line), GRK4 (yellow dashed line). Top picture: absolute error in the Hamiltonian function. Bottom picture: absolute error in the angular momentum.

We set $e = 0.6$ and $h = \mu/200$, and we integrate the problem over 10^5 periods. Setting $\mathbf{y} := (q_1, q_2, p_1, p_2)$, the error $\|\mathbf{y}_j - \mathbf{y}_0\|_1$ in the solution is computed at specific times equal to multiples of the period, that is at $t_j = 2\pi j$, with $j = 1, 2, \ldots$. The errors in the invariants have been computed at the mesh points $t_n = \pi n$, $n = 1, 3, 5, \ldots$.

Figures 1-2 report the results obtained by the four fourth-order methods. Figure 1 reports the absolute error in the numerical solution. In Figure 2, the top picture shows the absolute error in the Hamiltonian function while the absolute error in the angular momentum is drawn in the bottom picture.

As is expected, we can see a linear drift in the error $\|\mathbf{y}_j - \mathbf{y}_0\|_1$ as the time increases. In the other pictures, as is the case with the Euler-Maclaurin and Gauss methods, we can see that MDMP and MDTR methods guarantee a near conservation of the Hamiltonian function and the angular momentum. Notice that this latter quadratic invariant is precisely conserved (up to machine precision) by the Gauss R–K method due to its symplecticity property.

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AMS Subject Classification: 65L06, 65P10, 65D25

Felice IAVERNARO,
Department of Mathematics, University of BARI Aldo Moro
Via Orabona 4, 70125 Bari, ITALY
e-mail: `felice.iavernaro@uniba.it`

Francesca MAZZIA,
Department of Computer Science, University of BARI Aldo Moro
Via Orabona 4, 70125 Bari, ITALY
e-mail: `francesca.mazzia@uniba.it`

Lavoro pervenuto in redazione il 16-5-19.