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A simple framework for the derivation and analysis of effective one-step methods for ODEs ☆

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ABSTRACT

In this paper, we provide a simple framework to derive and analyse a class of one-step methods that may be conceived as a generalization of the class of Gauss methods. The framework consists in coupling two simple tools: firstly a local Fourier expansion of the continuous problem is truncated after a finite number of terms and secondly the coefficients of the expansion are computed by a suitable quadrature formula. Different choices of the basis lead to different classes of methods, even though we shall here consider only the case of an orthonormal polynomial basis, from which a large subclass of Runge–Kutta methods can be derived. The obtained results are then applied to prove, in a simplified way, the order and stability properties of Hamiltonian BVMs (HBVMs), a recently introduced class of energy preserving methods for canonical Hamiltonian systems (see [2] and references therein). A few numerical tests are also included, in order to confirm the effectiveness of the methods resulting from our analysis.

1. Introduction

One-step methods are widely used in the numerical solution of initial value problems for ordinary differential equations which, without loss of generality, we shall assume to be in the form:

$$y'(t) = f(y(t)), \quad t \in [0,T], \quad y(0) = y_0 \in \mathbb{R}^m. \tag{1}$$

In particular, we consider a very general class of effective one-step methods that can be led back to a local Fourier expansion of the continuous problem over the interval $[0,h]$, where h is the considered stepsize. In general, different choices of the basis result in different classes of methods, for which, however, the analysis turns out to be remarkably simple. Though the arguments can be extended to a general choice of the basis, we consider here only the case of a polynomial basis, obtaining a large subclass of Runge–Kutta methods, even though trigonometric or exponential fitted type bases (see, e.g. [1,9,14,16,18]) could be, in principle, considered. Usually, the order properties of such methods are studied through the classical theory of Butcher on rooted trees (see, e.g. [8, Chapter 3]), almost always resorting to the so called *simplifying assumptions* (see, e.g. [8, Section 321]). For the methods derived in the new framework (see Section 2), such analysis turns out to be greatly simplified. Similar arguments apply to the linear stability analysis of the methods, here easily discussed through the Lyapunov method. Then, we apply the same procedure to the case where (1) is a canonical Hamiltonian problem, i.e., a problem in the form:

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$$\frac{dy}{dt} = J\nabla H(y), \quad J = \begin{pmatrix} 0 & I_m \\ -I_m & 0 \end{pmatrix}, \quad y(0) = y_0 \in \mathbb{R}^{2m}, \tag{2}$$

where $H(y)$ is a smooth scalar function, thus obtaining, in Section 3, an alternative derivation of the recently introduced class of energy preserving methods called Hamiltonian BVMs (HBVMs, see [2–4] and references therein). A few numerical examples concerning such methods are then provided in Section 4, in order to make evident their potentialities. Some concluding remarks are then given in Section 5.

2. Local Fourier expansion of ODEs

Let us consider problem (1) restricted to the interval $[0,h]$:

$$y' = f(y), \quad t \in [0,h], \quad y(0) = y_0. \tag{3}$$

In order to make the arguments as simple as possible, we shall hereafter assume f to be analytical. Let us consider an orthonormal polynomial basis $\{\widehat{P}_j\}_{j=0}^{\infty}$ over the interval $[0,1]$: i.e., the shifted Legendre polynomials over the interval $[0,1]$, scaled in order to be orthonormal. Consequently,

$$\int_0^1 \widehat{P}_i(x)\widehat{P}_j(x)\mathrm{d}x = \delta_{ij}, \quad \deg \widehat{P}_j = j, \quad \forall\, i,j \geqslant 0,$$

where δ_{ij} is the Kronecker symbol. We can then rewrite (3) by expanding the right-hand side:

$$y'(ch) = \sum_{j=0}^{\infty} \widehat{P}_j(c)\gamma_j(y), \quad c \in [0,1]; \quad \gamma_j(y) = \int_0^1 \widehat{P}_j(\tau) f(y(\tau h))\mathrm{d}\tau. \tag{4}$$

The basic idea is now that of truncating the series after r terms, which turns (4)[2] into:

$$\omega'(ch) = \sum_{j=0}^{r-1} \widehat{P}_j(c)\gamma_j(\omega), \quad c \in [0,1]; \quad \gamma_j(\omega) = \int_0^1 \widehat{P}_j(\tau) f(\omega(\tau h))\mathrm{d}\tau. \tag{5}$$

By imposing the initial condition, one then obtains:

$$\omega(ch) = y_0 + h\sum_{j=0}^{r-1} \gamma_j(\omega) \int_0^c \widehat{P}_j(x)\mathrm{d}x, \quad c \in [0,1]. \tag{6}$$

Obviously, ω is a polynomial of degree at most r. The following question then naturally arises: *"how close are $y(h)$ and $\omega(h)$?"* The answer is readily obtained, by using the following preliminary result.

Lemma 1. *Let $g : [0,h] \to \mathbb{R}^m$ be of class $C^j([0,h])$.*[3] *Then $\int_0^1 \widehat{P}_j(\tau) g(\tau h) d\tau = O(h^j)$.*

Proof. Assume, for sake of simplicity, that $g(\tau h)$ can be expanded in Taylor series at the origin. Then, for all $j \geqslant 0$, by considering that $\widehat{P}_j$ is orthogonal to all polynomials of degree $n < j$:

$$\int_0^1 \widehat{P}_j(\tau) g(\tau h)\mathrm{d}\tau = \sum_{n=0}^{\infty} \frac{g^{(n)}(0)}{n!} h^n \int_0^1 \widehat{P}_j(\tau)\tau^n \mathrm{d}\tau = O(h^j).$$

For a given fixed $j \geqslant 0$, the above arguments can be easily adapted, by considering the Taylor expansion of g with remainder at the jth term, provided that g is of class $C^j([0,h])$. □

As a consequence, one has that (see (5)) $\gamma_j(\omega) = O(h^j)$. To express the dependence of the solutions of $y' = f(y)$ on the initial values, for any given $\tilde{t} \in [0,h]$, we will denote by $y(\cdot,\tilde{t},\tilde{y})$ the solution satisfying the initial condition $y(\tilde{t},\tilde{t},\tilde{y}) = \tilde{y}$.[4] Similarly, we set:

$$\Phi(s,\tilde{t},\tilde{y}) = \frac{\partial}{\partial \tilde{y}} y(s,\tilde{t},\tilde{y}), \tag{7}$$

also recalling the following standard result from the theory of ODEs:

$$\frac{\partial}{\partial \tilde{t}} y(s,\tilde{t},\tilde{y}) = -\Phi(s,\tilde{t},\tilde{y}) f(\tilde{y}). \tag{8}$$

[2] To simplify the notation, we avoid to adopt the more complete notation $\gamma_j(f(y),h)$ to denote the coefficients involved in the Fourier expansion.
[3] i.e., g has j continuous derivatives in the interval $[0,h]$.
[4] Clearly, since the problem is autonomous, then $y(s,\tilde{t},\tilde{y}) = y(s-\tilde{t},0,\tilde{y})$.

We can now state the following result, whose proof is essentially based on that of [15, Theorem 6.5.1 on pp. 165–166].

Theorem 1. *Let $y(ch)$ and $\omega(ch)$, $c \in [0,1]$, be the solutions of (4) and (5), respectively, satisfying the initial condition $y(0) = \omega(0) = y_0$. Then, $y(h) - \omega(h) = O(h^{2r+1})$.*

Proof. By virtue of Lemma 1 and (7) and (8), one has:[5]

$$\begin{aligned} y(h) - \omega(h) &= y(h,0,y_0) - y(h,h,\omega(h)) = -\int_0^h \frac{\mathrm{d}}{\mathrm{d}\tau} y(h,\tau,\omega(\tau))\mathrm{d}\tau = -\int_0^h \left(\frac{\partial}{\partial \bar{t}} y(h,\tau,\omega(\tau)) + \frac{\partial}{\partial \bar{y}} y(h,\tau,\omega(\tau))\omega'(\tau)\right)\mathrm{d}\tau \\ &= h\int_0^1 \Phi(h,ch,\omega(ch))(f(\omega(ch)) - \omega'(ch))\mathrm{d}c = h\int_0^1 \Phi(h,ch,\omega(ch))\left(\sum_{j=r}^{\infty} \gamma_j(\omega)\widehat{P}_j(c)\right)\mathrm{d}c \\ &= h\sum_{j=r}^{\infty}\left(\int_0^1 \widehat{P}_j(c)\Phi(h,ch,\omega(ch))\mathrm{d}c\right)\gamma_j(\omega) = h\sum_{j=r}^{\infty} O(h^j)O(h^j) = O(h^{2r+1}). \qquad \square \end{aligned}$$

The previous result reveals the extent to which the polynomial $\omega(t)$, solution of (5), approximates the solution $y(t)$ of the original problem (3) on the time interval $[0,h]$. Obviously, the value $\omega(h)$ may serve as the initial condition for a new IVP in the form (5) approximating $y(t)$ on the time interval $[h,2h]$. In general, setting $t_i = ih$, $i = 0,1,\ldots$, and assuming that an approximation $\omega(t)$ is available on the interval $[t_{i-2}, t_{i-1}]$, one can extend the approximation to the interval $[t_{i-1}, t_i]$ by solving the IVP:

$$\omega'(t_{i-1} + ch) = \sum_{j=0}^{r-1} \widehat{P}_j(c) \int_0^1 \widehat{P}_j(\tau) f(\omega(t_{i-1} + ch))\mathrm{d}\tau, \quad c \in [0,1], \tag{9}$$

the initial value $\omega(t_{i-1})$ having been computed at the preceding step. The approximation to $y(t)$ is thus extended on an arbitrary interval $[0,Nh]$, and the function $\omega(t)$ is a continuous piecewise polynomial. As a direct consequence of Theorem 1, we obtain the following straightforward result.

Corollary 1. *Let $T = Nh$, where $h > 0$ and N is an integer. The approximation to the solution of problem (1) by means of (9) at the grid-points $t_i = t_{i-1} + h$, $i = 1,\ldots,N$, with $\omega(t_0) = y_0$, is $O(h^{2r})$ accurate.*

We now want to compare the asymptotic behavior of $\omega(t)$ and $y(t)$ on the infinite length interval $[0,+\infty)$ in the case where f is linear or defines a canonical Hamiltonian problem. To this end we introduce the infinite sequence $(\omega_i) \equiv (\omega(t_i))$.

Remark 1. Though in general, the sequence (ω_i) cannot be formally regarded as the outcome of a numerical method, under special situations, this can be the case. For example, when f is a polynomial, the integrals in (5) may be explicitly determined and the IVP in (5) is evidently equivalent to a nonlinear system having as unknowns the coefficients of the polynomial ω expanded along a given basis (for example, the polynomial ω may be computed by means of the method of undetermined coefficients). This issue, as well as details about how to manage the integrals in the event that the integrands do not admit an analytical primitive function in closed form, will be thoroughly faced in Section 3.

Remark 2. We observe that a different choice of the orthonormal basis would, in general, modify the above arguments. In more details, for any given basis, a result analogous to Lemma 1 would be needed. The result of Theorem 1 is then modified accordingly. Different choices of the basis will be considered in future investigations.

2.1. Linear stability analysis

For the linear stability analysis, one needs to consider the celebrated test equation:

$$y' = \lambda y, \quad \Re(\lambda) \leqslant 0. \tag{10}$$

By setting

$$\lambda = \alpha + \mathrm{i}\beta, \quad y = x_1 + \mathrm{i}x_2, \quad x = (x_1, x_2)^T, \quad A = \begin{pmatrix} \alpha & -\beta \\ \beta & \alpha \end{pmatrix},$$

with i the imaginary unit, problem (10) can be rewritten as:

$$x' = Ax, \quad t \in [0,h], \quad x(0) \text{ given}. \tag{11}$$

[5] In the sequel, the notation such as $\frac{\partial}{\partial \bar{t}} y(h,\tau,\omega(\tau))$ will denote the partial derivative of $y(s,\bar{t},\bar{y})$ with respect to $\bar{t}$, evaluated at $s = h$, $\bar{t} = \tau$ and $\bar{y} = \omega(\tau)$ and analogously for the partial derivative of $y(s,\bar{t},\bar{y})$ with respect to $\bar{y}$.

Consequently, the corresponding truncated problem (5) becomes:

$$\omega'(ch) = A\sum_{j=0}^{r-1} \widehat{P}_j(c) \int_0^1 \widehat{P}_j(\tau)\nabla V(\omega(\tau h))\mathrm{d}\tau, \quad c \in [0,1], \tag{12}$$

where

$$V(x) = \frac{1}{2}x^T x \tag{13}$$

is a Lyapunov function for (11). From (12) and (13) one readily obtains:

$$\begin{aligned}\Delta V(\omega(0)) &= V(\omega(h)) - V(\omega(0)) = h\int_0^1 \nabla V(\omega(\tau h))^T \omega'(\tau h)\mathrm{d}\tau \\ &= h\sum_{j=0}^{r-1}\left[\int_0^1 \widehat{P}_j(\tau)\nabla V(\omega(\tau h))\mathrm{d}\tau\right]^T A\left[\int_0^1 \widehat{P}_j(\tau)\nabla V(\omega(\tau h))\mathrm{d}\tau\right] = \alpha h\sum_{j=0}^{r-1}\left\|\int_0^1 \widehat{P}_j(\tau)\omega(\tau h)\mathrm{d}\tau\right\|_2^2.\end{aligned}$$

The last equality follows by taking the symmetric part of A. We observe that:

$$\omega \neq 0 \Rightarrow \sum_{j=0}^{r-1}\left\|\int_0^1 \widehat{P}_j(\tau)\omega(\tau h)\mathrm{d}\tau\right\|_2^2 > 0,$$

since, conversely, this would imply $\omega(ch) = \rho\cdot\widehat{P}_r(c)$ for a suitable $\rho \neq 0$ and, therefore (from (12)), $\widehat{P}_r' \equiv 0$ which is clearly false. Thus, for a generic $y_0 \neq 0$,

$$\Delta V(\omega(0)) < 0 \Longleftrightarrow \Re(\lambda) < 0 \quad \text{and} \quad \Delta V(\omega(0)) = 0 \Longleftrightarrow \Re(\lambda) = 0.$$

Again, the above computation can be extended to any interval $[t_{i-1}, t_i]$ and, from the discrete version of the Lyapunov theorem (see, e.g. [15, Th. 4.8.3 on p. 108]), we have that the sequence ω_i tends to zero if and only if $\Re(\lambda) < 0$, while it remains bounded whenever $\Re(\lambda) = 0$, whatever is the stepsize $h > 0$ used. The following result is thus proved.

Theorem 2. *The continuous solution $y(t)$ of (10) and its discrete approximation ω_i have the same stability properties, for any choice of the stepsize $h > 0$.*

2.2. The Hamiltonian case

For Hamiltonian problems in the form (2), the approximation provided by the polynomial ω in (5) and (6) inherits a very important property of the continuous problem, i.e., energy conservation. Indeed, it is very well known that for the exact solution of (2) one has:

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

due to the fact that matrix J is skew-symmetric. Consequently, $H(y(t)) = H(y_0)$ for all t. For the truncated Fourier problem, the following result holds true.

Theorem 3. *$H(\omega(h)) = H(\omega(0)) \equiv H(y_0)$.*

Proof. From (5), considering that $f(\omega) = J\nabla H(\omega)$ and $J^T J = I$, one obtains:

$$\begin{aligned}H(\omega(h)) - H(y_0) &= h\int_0^1 \nabla H(\omega(\tau h))^T \omega'(\tau h)\mathrm{d}\tau = h\int_0^1 \nabla H(\omega(\tau h))^T \sum_{j=0}^{r-1}\widehat{P}_j(\tau)\gamma_j(\omega)\mathrm{d}\tau \\ &= h\sum_{j=0}^{r-1}\left(\int_0^1 \nabla H(\omega(\tau h))\widehat{P}_j(\tau)\mathrm{d}\tau\right)^T \gamma_j(\omega) = h\sum_{j=0}^{r-1}\gamma_j(\omega)^T J\gamma_j(\omega) = 0,\end{aligned}$$

since J is skew-symmetric. □

3. Discretization

Clearly, the integrals in (5), if not directly computable, need to be numerically approximated. This can be done by introducing a quadrature formula based at $k \geqslant r$ abscissae c_i, thus obtaining an approximation to (5):

$$u'(ch) = \sum_{j=0}^{r-1} \widehat{P}_j(c) \sum_{\ell=1}^{k} b_\ell \widehat{P}_j(c_\ell) f(u(c_\ell h)), \quad c \in [0,1], \tag{14}$$

where the b_ℓ are the quadrature weights, and u is the resulting polynomial, of degree at most r, approximating ω. It can be obtained by solving a discrete problem in the form:

$$u'(c_i h) = \sum_{j=0}^{r-1} \widehat{P}_j(c_i) \sum_{\ell=1}^{k} b_\ell \widehat{P}_j(c_\ell) f(u(c_\ell h)), \quad i = 1, \dots, k. \tag{15}$$

Let q be the order of the formula, i.e., let it be exact for polynomials of degree less than q (we observe that $q \geqslant k \geqslant r$). Clearly, since we assume f to be analytical, choosing k large enough, along with a suitable choice of the nodes c_i, allows us to approximate the given integral to any degree of accuracy, even though, when using finite precision arithmetic, it suffices to approximate it to machine precision. We observe that, since the quadrature is exact for polynomials of degree $q-1$, its remainder depends on the q-th derivative of the integrand with respect to τ. Consequently, considering that $\widehat{P}_j^{(i)}(c) \equiv 0$, for $i > j$, one has:

$$\Delta_j(h) \equiv \int_0^1 \widehat{P}_j(\tau) f(u(\tau h)) \mathrm{d}\tau - \sum_{\ell=1}^{k} b_\ell \widehat{P}_j(c_\ell) f(u(c_\ell h)) = O(h^{q-j}), \tag{16}$$

$j = 0, \dots, r-1$. Thus, (14) is equivalent to the ODE,

$$u'(ch) = \sum_{j=0}^{r-1} \widehat{P}_j(c) \Big(\gamma_j(u) - \Delta_j(h) \Big), \quad c \in [0,1], \quad \gamma_j(u) = \int_0^1 \widehat{P}_j(\tau) f(u(\tau h)) \mathrm{d}\tau, \tag{17}$$

with $u(0) = y_0$, in place of (5). The following result then holds true.

Theorem 4. *Under the above hypotheses: $y(h) - u(h) = O(h^{p+1})$, with $p = \min(q, 2r)$.*

Proof. The proof is quite similar to that of Theorem 1; by virtue of Lemma 1 and (16) and (17), one obtains:

$$\begin{aligned}
y(h) - u(h) &= y(h,0,y_0) - y(h,h,u(h)) = -\int_0^h \frac{\mathrm{d}}{\mathrm{d}\tau} y(h,\tau,u(\tau)) \mathrm{d}\tau = -\int_0^h \left(\frac{\partial}{\partial \tilde{t}} y(h,\tau,u(\tau)) + \frac{\partial}{\partial \tilde{y}} y(h,\tau,u(\tau)) u'(\tau) \right) \mathrm{d}\tau \\
&= h \int_0^1 \Phi(h,ch,u(ch)) (f(u(ch)) - u'(ch)) \mathrm{d}c = h \int_0^1 \Phi(h,ch,u(ch)) \left(\sum_{j=0}^{r-1} \widehat{P}_j(c) \Delta_j(h) + \sum_{j=r}^{\infty} \gamma_j(u) \widehat{P}_j(c) \right) \mathrm{d}c \\
&= h \sum_{j=0}^{r-1} \left(\int_0^1 \widehat{P}_j(c) \Phi(h,ch,u(ch)) \mathrm{d}c \right) \Delta_j(u) + h \sum_{j=r}^{\infty} \left(\int_0^1 \widehat{P}_j(c) \Phi(h,ch,u(ch)) \mathrm{d}c \right) \gamma_j(u) \\
&= h \sum_{j=0}^{r-1} O(h^j) O(h^{q-j}) + h \sum_{j=r}^{\infty} O(h^j) O(h^j) = O(h^{q+1}) + O(h^{2r+1}). \qquad \square
\end{aligned}$$

As an immediate consequence, one has the following result.

Corollary 2. *Let q be the order of the quadrature formula defined by the abscissae $c_1, \dots, c_k$. Then, the order of the method (15) for approximating (1), with $y_1 = u(h)$, is $p = \min(q, 2r)$.*

Concerning the linear stability analysis, Theorem 2 implies that method (15) is perfectly A-stable[6] as soon as the condition $q \geqslant 2r$ is satisfied. In fact, in such a case, the quadrature formula based upon the abscissae $c_1, \dots, c_k$ is exact when the integrand is a polynomial of degree at most $2r-1$ and hence will match the integrals appearing in (12).

In the case $r = 1$, the above results apply to the methods in [12] (see also [13]).

3.1. Runge–Kutta formulation

By setting, as usual, $u_i = u(c_i h),\ u_i' = u'(c_i h),\ f_i = f(u_i),\ i = 1, \dots, k$, (15) can be rewritten as:

$$u_i = y_0 + h \sum_{j=0}^{r-1} \int_0^{c_i} \widehat{P}_j(\tau) \mathrm{d}\tau \sum_{\ell=1}^{k} b_\ell \widehat{P}_j(c_\ell) f_\ell, \quad i = 1, \dots, k. \tag{18}$$

Moreover, since $q \geqslant r \geqslant \deg u$, one has $y_1 = u(h) \equiv y_0 + h \sum_{\ell=1}^{k} b_\ell u_\ell'$. Consequently, the methods which Corollary 2 refers to are the subclass of k-stage Runge–Kutta methods with the following tableau:

[6] i.e., its absolute stability region coincides with the left-half complex plane, $\mathbb{C}^-$, [7].

$$\begin{array}{c|c} c_1 & \\ \vdots & A = (a_{ij}) \equiv \left(b_j \sum_{\ell=0}^{r-1} \widehat{P}_\ell(c_j) \int_0^{c_i} \widehat{P}_\ell(\tau)\mathrm{d}\tau \right). \\ c_k & \\ \hline & b_1 \quad \ldots \quad b_k \end{array} \tag{19}$$

In particular, in [5] it has been proved that when the nodes c_i coincide with the k Gauss points on the interval $[0,1]$, then:

$$A = \mathcal{A}\mathcal{P}\mathcal{P}^T\Omega, \tag{20}$$

where $\mathcal{A} \in \mathbb{R}^{k\times k}$ is the matrix in the Butcher tableau of the k-stage Gauss method, $\mathcal{P} = (\widehat{P}_{j-1}(c_i)) \in \mathbb{R}^{k\times r}$, and $\Omega = \mathrm{diag}(b_1,\ldots,b_k)$. In such a way, when $k = r$, one obtains the classical r-stage Gauss collocation method. Consequently, (19) can be regarded as a generalization of the classical Runge–Kutta collocation methods, (15) being interpreted as *extended collocation conditions*.

3.2. Hamiltonian Boundary Value Methods (HBVMs)

When considering a canonical Hamiltonian problem (2), the discretization of the integrals appearing in (5) by means of a Gaussian formula at k nodes results in the HBVM (k,r) methods introduced in [4].[7] For such methods we derive, in a novel way with respect to [2–4], the following result.

Corollary 3. *For all $k \geqslant r$, the HBVM (k,r) is perfectly A-stable and has order $2r$. The method is energy conserving for all polynomial Hamiltonians of degree not larger than $2k/r$.*

Proof. The result on the order and linear stability easily follow from Corollary 2 and the discussion in the subsequent text. Concerning the energy conservation property, one has:

$$\begin{aligned} H(u(h)) - H(y_0) &= h\int_0^1 \nabla H(u(\tau h))^T u'(\tau h)\mathrm{d}\tau = h\int_0^1 \nabla H(u(\tau h))^T \sum_{j=0}^{r-1} \widehat{P}_j(\tau) \sum_{\ell=1}^{k} b_\ell \widehat{P}_j(c_\ell) J \nabla H(u(c_\ell h))\mathrm{d}\tau \\ &= h\sum_{j=0}^{r-1} \left[\int_0^1 \widehat{P}_j(\tau)\nabla H(u(\tau h))\mathrm{d}\tau\right]^T J \left[\sum_{\ell=1}^{k} b_\ell \widehat{P}_j(c_\ell)\nabla H(u(c_\ell h))\right] = 0, \end{aligned}$$

provided that

$$\int_0^1 \widehat{P}_j(\tau)\nabla H(u(\tau h))\mathrm{d}\tau = \sum_{\ell=1}^{k} b_\ell \widehat{P}_j(c_\ell)\nabla H(u(c_\ell h)). \tag{21}$$

In the case where H is a polynomial of degree ν, this is true provided that the integrand is a polynomial of degree at most $2k-1$. Consequently, $\nu r - 1 \leqslant 2k - 1$, i.e., $\nu \leqslant 2k/r$. □

For general Hamiltonian problems, by using the same argument as in the previous proof, one concludes that:

$$H(u(h)) - H(y_0) = O(h^{2k+1}), \tag{22}$$

that is, the Hamiltonian is approximated with order $2k$ on any finite interval. As a consequence, by considering the limit as $k \to \infty$ we recover formulae (5), which have been called *HBVM (∞,r)* (or, more in general, *∞-HBVMs*) [2,4]: in particular, (6) is nothing but the *Master Functional Equation* in [2,4].

Remark 3. We observe that, due to what was shown in [4], the above analysis and arguments apply to the methods in [10], which are obtained by using the Lagrange basis, instead of the Legendre one.

Remark 4. In the case of polynomial Hamiltonian systems, if (21) holds true for $k = k^*$, then:

$$\mathrm{HBVM}(k,r) \equiv \mathrm{HBVM}(k^*,r) \equiv \mathrm{HBVM}(\infty,r), \quad \forall\, k \geqslant k^*.$$

That is, (14) coincides with (5), for all $k \geqslant k^*$. In the non-polynomial case, the previous conclusions continue "practically" to hold, provided that the integrals are approximated within machine precision, i.e., by considering k large enough (see (22)). However, we observe that, whatever the choice of k, matrix A in (20) has constant rank r. This implies that the k equations defining the stages may be suitably arranged in $k - r$ linear and r nonlinear equations. An important consequence is that the

[7] A different discretization, based at $k+1$ Lobatto abscissae, was previously considered in [3].

computational cost associated with the method is practically independent of the number k of the quadrature nodes (see, e.g. [6]) and hence a practical energy conservation may be attained for any smooth Hamiltonian problem.

4. Numerical tests

We here provide a few numerical tests, showing the effectiveness of HBVMs, namely of the methods obtained in the new framework, when the problem (1) is in the form (2).

4.1. The Kepler problem

We consider at first the Kepler problem, with Hamiltonian:

$$H([q_1,q_2,p_1,p_2]^T) = \frac{1}{2}(p_1^2+p_2^2) - (q_1^2+q_2^2)^{-\frac{1}{2}}.$$

When started at

$$(1-e,0,0,\sqrt{(1+e)/(1-e)})^T, \quad e\in[0,1),$$

it has an elliptic periodic orbit of period 2π and eccentricity e. When e is not close to 1, the problem is efficiently solved by using a constant stepsize. However, it becomes more and more difficult as $e\to 1$, so that a variable-step integration would be more appropriate in this case. We first compare the following 6-th order methods for solving such a problem over a 1000 periods interval:

- HBVM (3,3), i.e., the GAUSS6 method, which is a symmetric and symplectic method;
- HBVM (4,3), which is symmetric [3] but not symplectic nor energy preserving, since the Gauss quadrature formula of order 8 is not enough accurate, for this problem;
- HBVM (9,3), which is *practically* energy preserving, since the Gauss formula of order 18 is accurate within machine precision, for this problem, and for the used stepsize.

The two plots in Fig. 1 report the results obtained when $e = 0.6$ and a constant stepsize is used: as one can see from the left plot, the Hamiltonian error is 6th-order accurate for GAUSS6, and 8th-order accurate for HBVM (4,3) (according to (22)); conversely, the energy is (practically) conserved for the HBVM (9,3) method. On the other hand, from the right plot one obtains that all methods exhibit the same order (i.e., 6), with the error constant of the HBVM (4,3) and HBVM (9,3) methods much smaller than that of the symplectic GAUSS6 method.

Conversely, when $e = 0.99$, we consider a variable stepsize implementation with the following *standard* mesh-selection strategy:

$$h_{new} = 0.85\cdot h_n\left(\frac{tol}{err_n}\right)^{1/(p+1)}, \tag{23}$$

where $p = 6$ is the order of the method, tol is the prescribed tolerance, h_n is the current stepsize, and err_n is an estimate of the local error. According to what stated in the literature, this is not an advisable choice for symplectic methods, for which a *drift*

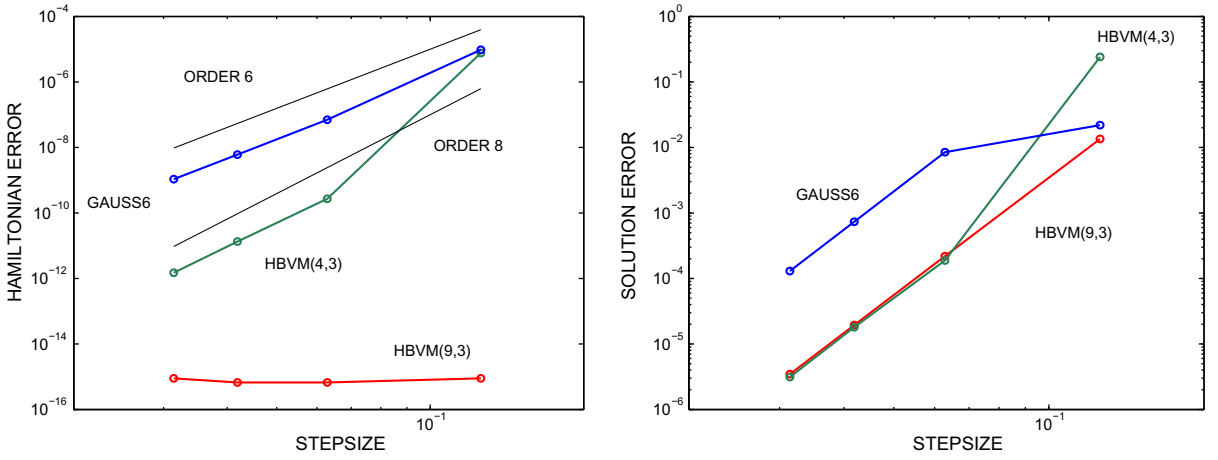

Fig. 1. Kepler problem, $e = 0.6$; Hamiltonian (left plot) and solution (right plot) errors over 1000 periods with a constant stepsize.

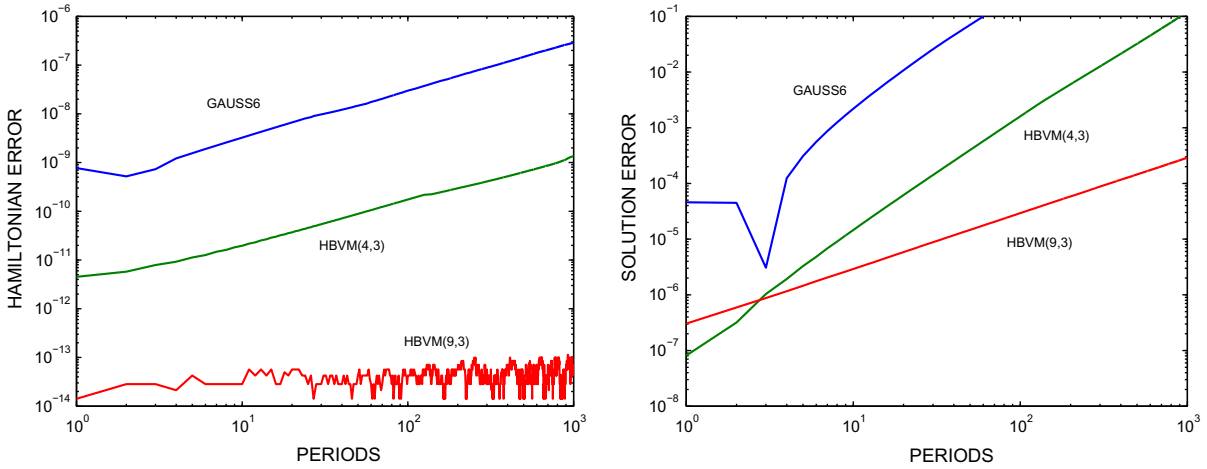

Fig. 2. Kepler problem, $e = 0.99$; Hamiltonian (left plot) and solution (right plot) errors over 1000 periods with a variable stepsize, $tol = 10^{-12}$. Note that, in contrast to HBVM (9,3), HBVM (4,3) is not energy preserving.

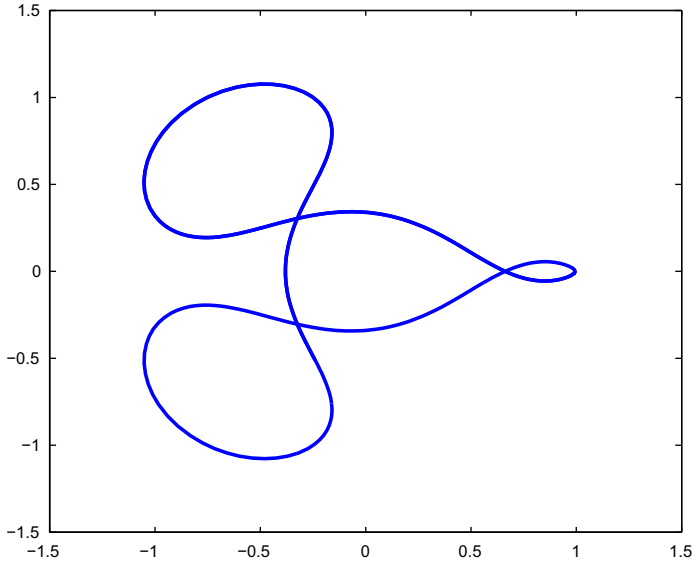

Fig. 3. Restricted three-body problem, Arenstorf's orbit corresponding to (24).

Table 1
Numerical solution of the Arenstorf's orbit starting at (24) by using $tol = 10^{-12}$ and $h_0 = 10^{-5}$.

Periods	GAUSS6				HBVM (9,3)			
	Solution error	Hamiltonian error	Mesh points	Fixed-point iterations	Solution error	Hamiltonian error	Mesh points	Fixed-point iterations
1	3.60e−8	5.84e−11	528	4315	2.82e−7	1.40e−14	435	3780
2	2.62e−5	9.37e−11	525	4301	1.70e−6	1.58e−14	432	3808
3	8.95e−3	1.29e−10	525	4302	5.60e−3	2.62e−14	432	3814
4	1.66e0	1.69e−10	628	5098	7.28e−1	2.93e−14	410	3612

in the Hamiltonian appears, and a *quadratic* error growth in the solution is experienced, as is confirmed by the two plots in Fig. 2. The same happens for the method HBVM (4,3), which is symmetric but not energy conserving. Conversely, for the (practically) energy conserving method HBVM (9,3), *no drift* in the Hamiltonian occurs and a *linear* error growth in the solution is observed.

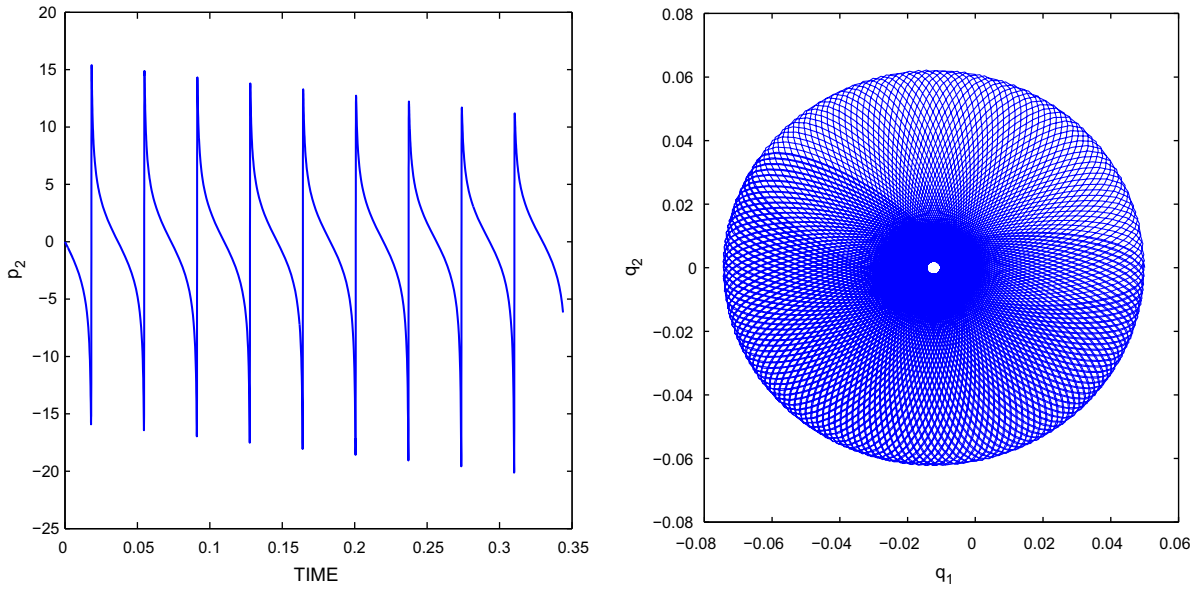

Fig. 4. Restricted three-body problem, orbit starting at (25).

Even though we do not discuss here the actual implementation of the methods, for sake of completeness we mention that in the numerical tests the error estimate err_n, to be used in (23), has been obtained as follows:

- for the GAUSS6 method, at each step we also compute the approximate step by means of the GAUSS8 (i.e., HBVM (4,4)) method;
- for the HBVM $(k,3)$ method, we also compute the approximate step by means of the 8-th order HBVM $(k,4)$ method, $k = 4,9$.

In the latter case, the (approximate) solution is obtained by using the same stages as those used by the corresponding 6th order method, so that its computation is inexpensive.

4.2. The planar restricted three-body problem

This problem [17, pages 115ff] describes the motion of three bodies: two *primaries* with masses μ and $1-\mu$, evolving in a plane, and a third (virtually massless) body called planetoid, which does not affect the motion of the primaries. The primaries move in circular orbits, and the massless body is assumed to move in the same plane of the primaries. The problem is now to find the trajectory of the massless body. The system is described on a rotating frame with the center of mass located at the origin and the two primaries placed at the points $(0,1-\mu)$ and $(0,-\mu)$. In such a case, the Hamiltonian is given by:

$$H(q,p) = \frac{1}{2}(p_1^2+p_2^2) + p_1q_2 - p_2q_1 - \frac{1-\mu}{\rho_1} - \frac{\mu}{\rho_2},$$

where

$$\rho_1^2 = (q_1+\mu)^2 + q_2^2, \quad \rho_2^2 = (q_1-1+\mu)^2 + q_2^2.$$

With this Hamiltonian, the problem can be cast in canonical form. Moreover, there exist initial values such that the solution is periodic with period T. They are known as "Arenstorf orbits". One such orbit (see Fig. 3) is obtained with the data (adapted from [11, page 186]):

$$\begin{aligned} &\mu = 0.012277471, \quad T = 11.124340337266085134999734047,\\ &q_1(0) = 0.994, \quad q_2(0) = p_1(0) = 0, \quad p_2(0) = -1.037732629557336835730205792 4. \end{aligned} \tag{24}$$

The computation of this orbit is numerically challenging since it passes very close to one of the singular points of the problem and even a small perturbation would make the periodic motion of the planetoid change drastically. As a consequence, the use of a constant stepsize would prove highly inefficient (so that a variable stepsize is recommended) and anyway multiple periods are difficult to be recovered numerically. In Table 1 we list the results obtained by using the 6th-order Gauss method (GAUSS6) and the HBVM (9,3) method, by using the same variable stepsize strategy (23), with $tol = 10^{-12}$ and initial

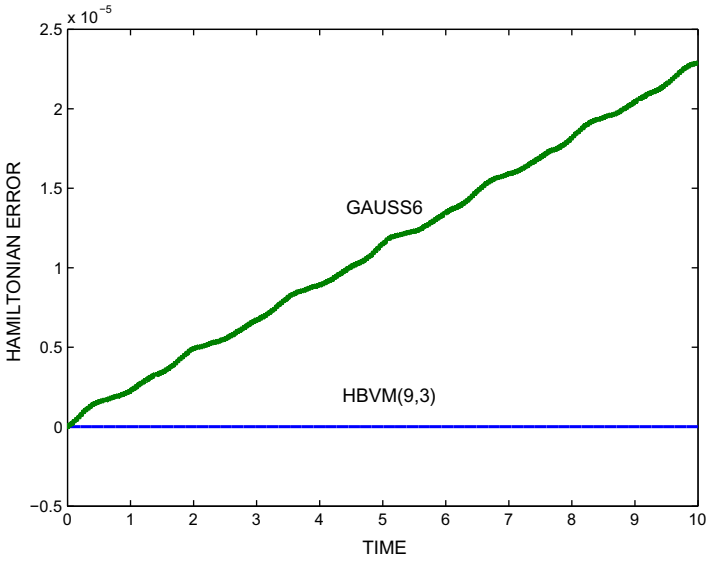

Fig. 5. Restricted three-body problem, orbit starting at (25); Hamiltonian error when using $tol = 10^{-10}$ and $h_0 = 10^{-5}$.

Table 2
Restricted three-body problem, orbit starting at (25); statistics at $T = 10$ when using $tol = 10^{-10}$ and $h_0 = 10^{-5}$.

Method	GAUSS6	HBVM (9,3)
Hamiltonian error	2.3e−05	3.0e−13
Solution error	2.41e−3	1.35e−6
Mesh-points	38302	32474
Fixed-point iterations	339364	311745

stepsize $h_0 = 10^{-5}$. The behavior of the two methods is conclusively similar, even though the latter method is able to obtain a more accurate solution by using a smaller number of mesh-points and requiring less fixed-point iterations per period. We arrive at a very different conclusion if we consider, instead of (24), the following set of data (the parameter μ is kept fixed):

$$q_1(0) = 0.05, \quad q_2(0) = p_1(0) = 0, \quad p_2(0) = 1. \tag{25}$$

Also in this case, a constant stepsize turns out to be very inefficient, because $p_1(t)$ and $p_2(t)$ exhibit "spikes" with a periodicity of about $3.6 \cdot 10^{-2}$, as is shown in the left plot of Fig. 4. On the other hand, the solution seems to lie on a torus, as one infers from the right plot of the same figure. We approximate the orbit starting at (25) up to $T = 10$ by using the GAUSS6 and HBVM (9,3) methods, with tolerance $tol = 10^{-10}$ and initial stepsize $h_0 = 10^{-5}$. A "reference" solution with a more accurate method (HBVM (10,5), used with tolerance $tol = 10^{-13}$) has been also computed, in order to compare the accuracy of the previous methods. As one may see from the plot in Fig. 5 the numerical Hamiltonian has a drift for the GAUSS6 method, whereas it is practically conserved for the HBVM (9,3) method. Table 2 contains some statistics, showing that the HBVM (9,3) method turns out to be more efficient than the GAUSS6 method, since it requires less mesh-points (as well as less fixed-point iterations) providing a more accurate solution, without drift in the numerical Hamiltonian.

5. Conclusions

In this paper, we have presented a general framework for the derivation and analysis of effective one-step methods, which is based on a local Fourier expansion of the problem at hand. In particular, when the chosen basis is a polynomial one, we obtain a large subclass of Runge–Kutta methods, which can be regarded as a generalization of Gauss collocation methods.

When dealing with canonical Hamiltonian problems, the methods coincide with the recently introduced class of energy preserving methods named HBVMs. A few numerical tests seem to show that such methods have interesting potentialities when compared with symplectic, or symmetric but non energy conserving, methods.

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