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# Recent Advances in the Numerical Solution of Conservative Problems

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**Abstract.** The numerical solution of conservative problems, i.e., problems characterized by the presence of constants of motion, is of great interest in the computational practice. Such problems, indeed, occur in many real-life applications, ranging from the nano-scale of molecular dynamics to the macro-scale of celestial mechanics. Often, they are formulated as Hamiltonian problems. Concerning such problems, recently the energy conserving methods named Hamiltonian Boundary Value Methods (HBVMs) have been introduced. In this paper we review the main facts about HBVMs, as well as the existing connections with other approaches to the problem. A few new directions of investigation will be also outlined. In particular, we will place emphasis on the last contributions to the field of Prof. Donato Trigiante, passed away last year.

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## INTRODUCTION

The numerical solution of conservative problems is an active field of investigation, dealing with the geometrical properties of the discrete vector field induced by the numerical methods, aimed to reproduce corresponding geometrical properties of the continuous one. Because of this reason, it has become customary to refer to this field of investigation as *geometric integration*, even though this concept can be led back to the early work of G. Dahlquist on differential equations, aimed to reproduce the asymptotic stability of equilibria for the trajectories produced by the numerical methods, resulting in the well-known linear stability analysis of the methods (see, e.g., [16]).

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

$$y' = J\nabla H(y), \qquad y(t_0) = y_0 \in \mathbb{R}^{2m}, \tag{1}$$

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

$$H(y(t)) \equiv H(y_0), \qquad \forall t \geq t_0,$$

for the solution of (1). Often, the Hamiltonian $H$ is also called the *energy*, since for isolated mechanical systems it has the physical meaning of total energy. Consequently, *energy conservation* is an important feature in the simulation of such problems. For the continuous dynamical system, it can be shown that energy conservation derives from the property of *symplecticity* of the map (see, e.g., [25]).

Concerning the numerical integration of (1), two main lines of investigation have been the definition and the study of *symplectic* methods and *energy-conserving* methods, respectively. This reflects the fact that the symplecticity of the map associated with (1) and energy conservation are the most relevant features characterizing a Hamiltonian system.

Symplectic methods can be found in early work of Gröbner (see, e.g., [27]). Symplectic Runge–Kutta methods have been then studied by Feng Kang [23], Suris [39], and Sanz Serna [38]. Such methods are obtained by imposing that the discrete map, associated with a given numerical method, is symplectic, as is the continuous one. Since for the continuous map symplecticity implies energy-conservation, then one expects that something similar happens for the discrete map as well. As a matter of fact, under suitable assumptions, it can be proved that, when a symplectic method is used with a constant step-size, the numerical solution satisfies a perturbed Hamiltonian problem, thus providing a quasi-conservation property over "exponentially long times" [1]. Even though this is an interesting feature, nonetheless, it constitutes a somewhat weak stability result since, in general, it doesn't extend to infinite intervals.

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

The very first attempts to face this problem were based on projection techniques coupled with standard non conservative numerical methods. However, it is well-known that this approach suffers from many drawbacks, in that this is usually not enough to correctly reproduce the dynamics (see, e.g., [29, p. 111]).

A completely new approach is represented by *discrete gradient methods*, which are based upon the definition of a discrete counterpart of the gradient operator, so that energy conservation of the numerical solution is guaranteed at each step and for any choice of the integration step-size [26, 36].

A different approach is based on the concept of *time finite element methods* [31], where one finds local Galerkin approximations on each subinterval of a given mesh of size $h$ for the equation (1). This, in turn, has led to the definition of energy-conserving Runge–Kutta methods [2, 3, 40].

A partially related approach is given by *discrete line integral methods* [32, 33, 34], where the key idea is to exploit the relation between the method itself and the *discrete line integral*, i.e., the discrete counterpart of the the line integral in conservative vector fields. This, in turn, allows exact conservation for polynomial Hamiltonians of arbitrarily high-degree, resulting in the class of methods later named *Hamiltonian Boundary Value Methods (HBVMs)*, which have been developed in a series of papers [7, 8, 6, 9, 10, 11, 12, 13].

Another approach, strictly related to the latter one, is given by the *Averaged Vector Field* method [37, 19] and its generalizations [28], which have been also analysed in the framework of B-series [20] (i.e., methods admitting a Taylor expansion with respect to the step-size).

With these premises, in the next section we recall the basic facts about HBVMs and its generalizations. Later on, we shall sketch a further approach leading to the definition of methods which are able to reproduce, to some extent, *both* the properties of symplecticity and energy conservation. Major emphasis will be placed on the contributions [7, 8, 9, 10, 11, 12, 13, 14, 15] to the field by Prof. Donato Trigiante, one of the leading Italian numerical analysts, passed away last year.

## HAMILTONIAN BOUNDARY VALUE METHODS

The basic idea HBVMs rely on is very simple. Indeed, one has that energy conservation for the solution of problem (1) follows as well from the vanishing of the *line integral*

$$H(y(t)) - H(y_0) = \int_{t_0}^{t} \nabla H(y(s))^T y'(s) \mathrm{d}s = 0, \qquad (2)$$

which is due to the fact that $y'(s) = J\nabla H(y(s))$, since $y$ is solution of (1), and $J^T = -J$. However, setting hereafter $t_0 = 0$, one can derive conservation at $t = h$ along any suitable path $\sigma(\cdot)$ such that

$$\begin{aligned} H(y_1) - H(y_0) \;&\equiv\; H(\sigma(h)) - H(\sigma(0)) \\ &= \int_0^h \nabla H(\sigma(s))^T \sigma'(s) \mathrm{d}s \qquad (3) \\ &= h \int_0^1 \nabla H(\sigma(\tau h))^T \sigma'(\tau h) \mathrm{d}\tau \;=\; 0. \end{aligned}$$

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

$$\sigma'(ch) = \sum_{j=0}^{s-1} \gamma_j P_j(c), \qquad c \in [0,1]. \qquad (4)$$

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

$$\sigma(ch) = y_0 + h \sum_{j=0}^{s-1} \gamma_j \int_0^c P_j(\tau) \mathrm{d}\tau, \qquad c \in [0,1]. \quad (5)$$

Moreover, by further imposing the vanishing of the line integral as in (3), one gets:

$$\begin{aligned} 0 \;&=\; \int_0^1 \nabla H(\sigma(\tau h))^T \sum_{j=0}^{s-1} \gamma_j P_j(\tau) \mathrm{d}\tau \\ &=\; \sum_{j=0}^{s-1} \left( \int_0^1 \nabla H(\sigma(\tau h)) P_j(\tau) \mathrm{d}\tau \right)^T \gamma_j. \end{aligned}$$

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

$$\gamma_j = \eta_j J \int_0^1 \nabla H(\sigma(\tau h)) P_j(\tau) \mathrm{d}\tau, \quad j = 0, \ldots, s-1, \quad (6)$$

for suitable scalars $\{\eta_j\}$. In particular, if the basis is orthogonal with respect to the scalar product

$$(f,g) = \int_0^1 f(\tau) g(\tau) \mathrm{d}\tau,$$

then

$$\eta_j = \left( \int_0^1 P_j^2(\tau) \mathrm{d}\tau \right)^{-1}, \quad j = 0, \ldots, s-1.$$

Hereafter, we shall consider the case where the polynomial basis is given by the Legendre polynomials, shifted

on the interval $[0,1]$, and scaled so that they are orthonormal:

$$\int_0^1 P_i(c)P_j(c)\mathrm{d}c = \delta_{ij}, \qquad \forall i,j \geq 0, \tag{7}$$

with $\delta_{ij}$, the Kroneckher symbol. Consequently,

$$\eta_j = 1, \qquad \forall j \geq 0. \tag{8}$$

More precisely, we are dealing with the following family of polynomials:

$$\begin{aligned} P_0(\tau) &\equiv 1, \qquad P_1(\tau) = \sqrt{3}\,(2\tau-1), \\ P_{j+1}(\tau) &= (2\tau-1)\,\frac{2j+1}{j+1}\sqrt{\frac{2j+3}{2j+1}}P_j(\tau) - \\ &\quad \frac{j}{j+1}\sqrt{\frac{2j+3}{2j-1}}P_{j-1}(\tau), \quad j \geq 1. \end{aligned} \tag{9}$$

With this choice, the nonlinear system defining the unknown coefficients $\gamma_j$ becomes

$$\gamma_j = \int_0^1 P_j(\tau) f\left(y_0 + h\sum_{i=0}^{s-1}\gamma_i \int_0^\tau P_i(c)\mathrm{d}c\right)\mathrm{d}\tau, \qquad j = 0,\ldots,s-1. \tag{10}$$

By virtue of (7) and considering that $P_0(\tau) \equiv 1$, the approximation $y_1 \simeq y(h)$ is then given by

$$y_1 \equiv \sigma(h) = y_0 + h\gamma_0. \tag{11}$$

We stress, however, that formulae (10)–(11) do not represent an operative method unless the integrals therein are approximated by means of a suitable quadrature formula. For this purpose, let us consider the interpolation quadrature formula defined by the abscissae

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

and the corresponding weights $\{b_i\}$. The final shape of a HBVM method, denoted by HBVM$(k,s)$, is then obtained by replacing (10) with

$$\gamma_j = \sum_{\ell=1}^{k} b_\ell P_j(c_\ell) f\left(y_0 + h\sum_{i=0}^{s-1}\gamma_i \int_0^{c_\ell} P_i(c)\mathrm{d}c\right), \qquad j = 0,\ldots,s-1, \tag{12}$$

which is a system of $s$ nonlinear vector algebraic equations in the unknowns $\{\gamma_j\}$.

HBVMs admit several equivalent formulations each emphasizing specific features they share. For example, (12)–(11) is appropriate for their implementation on a computer since the number of unknowns is minimum (compare with (14) below). Moreover, efficient iterative procedures for solving the discrete problem (12) have been discussed in [11].

On the other hand, to better show that HBVMs form a subclass of Runge–Kutta methods, we will introduce a different (though equivalent) formulation. Substituting (6) into (5) (see (8)), we see that the polynomial $\sigma$ satisfies the following *Master Functional Equation* [9]:

$$\sigma(ch) = y_0 + h\sum_{j=0}^{s-1}\int_0^c P_j(s)\mathrm{d}s \int_0^1 P_j(\tau) f(\sigma(\tau h))\mathrm{d}\tau, \qquad c \in [0,1], \tag{13}$$

where we have set $f(\sigma) \equiv J\nabla H(\sigma)$. Setting

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

and exploiting the quadrature formulae introduced above to approximate the integrals, we can discretize (13) as

$$Y_i = y_0 + h\sum_{j=0}^{s-1}\int_0^{c_i} P_j(s)\mathrm{d}s \sum_{\ell=1}^{k} b_\ell P_j(c_\ell) f(Y_\ell), \qquad i = 1,\ldots,k, \tag{14}$$

with the new approximation given by (compare with (11))

$$y_1 = y_0 + h\sum_{i=1}^{s} b_i f(Y_i). \tag{15}$$

Evidently, equations (14)-(15) represent the following $k$-stage Runge–Kutta method,

$$\begin{array}{c|c} c_1 & \\ \vdots & \left(b_j \sum_{\ell=0}^{s-1} P_\ell(c_j) \int_0^{c_i} P_\ell(x)\mathrm{d}x\right)_{i,j=1,\ldots,k} \\ c_k & \\ \hline & b_1 \quad \ldots \quad b_k \end{array} \tag{16}$$

which, as mentioned earlier, defines the Runge–Kutta shape of a *HBVM*$(k,s)$ *method* [7, 8, 9].

It is obvious that the higher $k$, the higher the order of the quadrature, which can be maximized (order=2$k$) by placing the abscissae $\{c_i\}$ at the Gauss-Legendre nodes in $[0,1]$. In such a case, the Runge–Kutta method (16) can be proved to have order $2s$ for all $k \geq s$, and the quadrature formula involved in the discretization of (10) or (13) turns out to be exact for all polynomial Hamiltonians of degree no larger than

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

Cosequently, for such problems, energy conservation is precisely obtained.

For non polynomial but suitably regular Hamiltonians, the error in the energy turns out to be $O(h^{2k+1})$, thus implying a *practical* conservation, provided that $k$ is large enough [7, 9]. Indeed, on a computer, energy-conservation is practically obtained as soon as full machine accuracy is reached.

We observe that by increasing the number $k$ of the quadrature nodes, the number of stages of the method (16) increases as well. However, as one infers from (10), the problem can be reformulated so that its (block) dimension is $s$, independently of $k$. As a matter of fact, the coefficient matrix of the Runge–Kutta method (16) has always rank equal to $s$, independently of its size $k$ (see for example [12], where it is also shown that the $s$ nonzero eigenvalues of an HBVM$(k,s)$ are always the same, for all $k \geq s$). This implies that $k-s$ of its stages may be expressed as linear combinations of the remaining ones. This leads to a further formulation of HBVMS, which is sketched below. We set

$$Y_f = [Y_1^T, \ldots, Y_s^T]^T \quad \text{and} \quad Y_s = [Y_{s+1}^T, \ldots, Y_k^T]^T.$$

Then, we can express the latter vector as [7, 9]

$$Y_s = a \otimes y_0 + (C \otimes I) Y_f, \tag{17}$$

for suitable $a \in \mathbb{R}^{k-s}$ and $C \in \mathbb{R}^{(k-s)\times s}$. For this reason, the stages belonging to $Y_f$ are referred to as *fundamental stages* while those belonging to $Y_s$ are called *silent stages* (they are not to be regarded as unknowns).

The above argument shows that the nonlinear system (14) is equivalent to (17) coupled with

$$Y_f = e \otimes y_0 + h(B_1 \otimes I) F(Y_f) + h(B_2 \otimes I) F(Y_s), \tag{18}$$

where

$$\begin{aligned} e &= (1, \ldots, 1)^T \in \mathbb{R}^s, \\ F(Y_f) &= [f(Y_1)^T, \ldots, f(Y_s)^T]^T, \\ F(Y_s) &= [f(Y_{s+1})^T, \ldots, f(Y_k)^T]^T. \end{aligned}$$

Clearly, by substituting (17) into (18), one obtains a discrete problem of dimension $s$, only involving the fundamental stages, i.e.,

$$\begin{aligned} Y_f = \; & e \otimes y_0 + h(B_1 \otimes I) F(Y_f) + \\ & h(B_2 \otimes I) F\left(a \otimes y_0 + (C \otimes I) Y_f\right). \end{aligned}$$

We refer to [7, 9] for full details.

## Line Integral Methods

This basic approach can be extended to more general problems, such as Poisson problems [4], as well as to *any* conservative problem possessing any number of invariants [5]. We briefly sketch this last issue, since its derivation from the previous approach is quite straightforward. Indeed, let us suppose that a general ODE-IVPs,

$$y' = f(y), \qquad y(0) = y_0, \tag{19}$$

has $\nu$ (independent) smooth constants of motion:

$$L(y(t)) = L(y_0) \in \mathbb{R}^\nu, \qquad t \geq 0. \tag{20}$$

The basic idea is now that of modifying the form of the polynomial (4) as follows:

$$\sigma'(ch) = \sum_{j=0}^{s-1} \gamma_j P_j(c) + \phi_0 \alpha, \qquad c \in [0,1], \tag{21}$$

with (see (19)–(20))

$$\begin{aligned} \gamma_j &= \int_0^1 P_j(\tau) f(\sigma(\tau h)) \mathrm{d}\tau, \qquad j = 0, \ldots, s-1, \\ \phi_j &= \int_0^1 P_j(\tau) J_L^T(\sigma(\tau h)) \mathrm{d}\tau, \end{aligned} \tag{22}$$

($\phi_j$ has been defined in general for later use), where $J_L(y)$ denotes the Jacobian matrix of the vector function $L(y)$. The unknown vector $\alpha \in \mathbb{R}^\nu$ is computed by imposing

$$L(y_1) \equiv L(\sigma(h)) = L(y_0).$$

Consequently, considering that $P_0 \equiv 1$, (5) becomes

$$\sigma(ch) = y_0 + h \sum_{j=0}^{s-1} \gamma_j \int_0^c P_j(\tau) \mathrm{d}\tau + c\phi_0 \alpha, \qquad c \in [0,1]. \tag{23}$$

By imposing, as usual, the conservation through a line integral, one then obtains (see (21) and (22)):

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

Since the invariants are independent each other, matrix $\phi_0^T \phi_0 \in \mathbb{R}^{\nu\times\nu}$ is symmetric and positive definite, so that $\alpha$ is formally computed as the solution of the linear system

$$\left(\phi_0^T \phi_0\right) \alpha = -\sum_{j=0}^{s-1} \phi_j^T \gamma_j. \tag{24}$$

We observe that, actually, (24) is nonlinear, since both the coefficient matrix and the right-hand side do depend on the unknown solution (23). This latter is obtained by solving the system of equations (22) and (24).

This approach can be extended to *any* method for which the discrete solution admits a continuous extension of the form (4)–(5) such as, for example, collocation methods. For this reason, all such methods have been collectively named *line integral methods (LIMs)* in [5]. As an example, in [5] a fully conservative variant of the

Gauss methods is also shown, along with that of HBVMs. Clearly, also in this case, a *numerical method* is actually obtained only after that the integrals in (22) are conveniently approximated by using a quadrature formula. In such a case, similar arguments as those used for HBVMs can be repeated. The interested reader is referred to [5] for full details and examples of applications.

In [14], a generalization in a different direction has been considered. Exploiting again the definition of the discrete line integral, a two-step method with energy conservation properties has been introduced and analyzed. Starting from two initial approximations $y_0 = y(0)$ and $y_1 \approx y(h)$ to the solution of (1), a polynomial $\sigma(2ch)$, $c \in [0,1]$, of degree 2 is defined by imposing the two interpolation conditions,

$$\sigma(0) = y_0, \qquad \sigma(h) = y_1,$$

and, moreover, by imposing the conservation of the Hamiltonian at $y_2 \equiv \sigma(2h)$,

$$H(y_2) = H(y_0).$$

This is done via the line integral form (compare with (3)):

$$\begin{aligned} H(y_2) - H(y_0) \;&\equiv\; H(\sigma(2h)) - H(\sigma(0)) \\ &= \int_0^h \nabla H(\sigma(2s))^T \sigma'(2s)\mathrm{d}s \\ &= h\int_0^1 \nabla H(\sigma(2\tau h))^T \sigma'(2\tau h)\mathrm{d}\tau \;=\; 0. \end{aligned} \tag{25}$$

As usual, a corresponding numerical method is obtained by using a suitable quadrature formula. It can be shown that the method is fourth-order, provided that the two initial approximation are $O(h^5)$ accurate, and that the quadrature used has a suitably high degree of precision. We refer the reader to [14] for full details and related numerical experiments.

It is worth mentioning that this approach can be extended to any number of initial steps, as well as to methods of GLM type, by means of similar arguments: this will be the subject of future investigations.

## Low-rank symplectic Runge–Kutta methods

A noticeable extension of symplectic Gauss Legendre methods has been recently devised by K. Burrage and P.M. Burrage [17], starting from the Runge–Kutta formulation of HBVMs. Indeed, the Butcher tableau (16) of the HBVM$(k,s)$ can be re-written by considering the following relations between the Legendre polynomials (9) and their integrals:

$$\begin{aligned} \int_0^c P_0(\tau)\mathrm{d}\tau &= \xi_1 P_1(c) + \frac{1}{2}P_0(c), \\ \int_0^c P_j(\tau)\mathrm{d}\tau &= \xi_{j+1}P_{j+1}(c) - \xi_j P_{j-1}(c), \quad j \ge 1, \end{aligned} \tag{26}$$

where

$$\xi_j = \frac{1}{2\sqrt{4j^2-1}}, \quad j \ge 1. \tag{27}$$

Indeed, by introducing the matrices (see (9))

$$\mathscr{P}_r = \begin{pmatrix} P_0(c_1) & \dots & P_{r-1}(c_1) \\ \vdots & & \vdots \\ P_0(c_k) & \dots & P_{r-1}(c_k) \end{pmatrix} \in \mathbb{R}^{k\times r}, \tag{28}$$

for $r \ge 1$, and (see (27))

$$\hat{X}_s = \begin{pmatrix} \frac{1}{2} & -\xi_1 & & \\ \xi_1 & 0 & \ddots & \\ & \ddots & \ddots & -\xi_{s-1} \\ & & \xi_{s-1} & 0 \\ & & & \xi_s \end{pmatrix} \in \mathbb{R}^{s+1\times s}, \tag{29}$$

the vector $b \in \mathbb{R}^k$ with the quadrature weights, and the diagonal matrix

$$B = \mathrm{diag}(b),$$

one has that the Butcher matrix in (16) can be written as

$$\hat{A} = \mathscr{P}_{s+1}\hat{X}_s\mathscr{P}_s^T B. \tag{30}$$

In [17], the authors consider the following Butcher matrix, in place of (30),

$$A = \mathscr{P}_s X_s \mathscr{P}_s^T B, \tag{31}$$

with (compare with (29))

$$X_s = \begin{pmatrix} \frac{1}{2} & -\xi_1 & & \\ \xi_1 & 0 & \ddots & \\ & \ddots & \ddots & -\xi_{s-1} \\ & & \xi_{s-1} & 0 \end{pmatrix} \in \mathbb{R}^{s\times s}. \tag{32}$$

It can be easily shown that, provided that the quadrature has order at least $2s$, then the corresponding method has order $2s$ with the Butcher matrix of rank $s$ (as the underlying HBVM$(k,s)$) method), for all $k \ge s$. Moreover, it is straightforward to verify that the following criterion for symplecticity (see, e.g., [29]), derived from the algebraic stability properties of implicit Runge–Kutta methods [18, 22],

$$A^T B + BA = bb^T, \tag{33}$$

is satisfied. In particular, when $k = s$, and the nodes are placed at the Gauss points, then (31) provides the

Butcher matrix of the $s$-stage Gauss method. Consequently, the method (31) turns out to be symplectic for all $k \geq s$ though, in general, not energy-preserving, alike the underlying Gauss method.

The usefulness of such low-rank symplectic Runge–Kutta methods stems in their better approximation properties, when numerically solving stochastic ODEs with additive noise, with respect to the corresponding Gauss method [17]. Indeed, the higher number of stages allows for a better approximation of the involved stochastic integrals.

## SYMPLECTIC AND ENERGY-CONSERVING METHODS

We here report an overview, with some modifications, of what exposed in [15]. The goal is to devise a method that, when applied to the Hamiltonian system (1), possesses to some extent *both* the properties of symplecticity of the map and of energy-conservation.

In so doing, one has to cope with two non-existence results. The first [24] refers to non-integrable systems, that is systems that do not admit other independent first integrals different from the Hamiltonian function itself. According to the authors' words,

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

The second negative result [21] refers to B-series symplectic methods applied to general (not necessarily non-integrable) Hamiltonian systems:

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

The impossibility for a constant time-stepping algorithm to be at the same time symplectic and energy conserving has led to research into methods which could inherit both features in a weaker sense. This delicate aspect has been thoroughly faced in [35] where the authors prove the existence of *symplectic–energy–momentum integrators* by using time-adaptive steps. Indeed, for Runge–Kutta methods, the criterion of symplecticity (33) coincides with that of preserving all quadratic integrals (such as, for example, the total angular momentum, in isolated mechanical systems).

For this reason, modifications of the basic Gauss collocation methods have been researched, able to inherit both features. According to the previous remark, they have been named *Energy and QUadratic Invarian Preserving (EQUIP) methods* [15]. The starting point is the following decomposition of the coefficient matrix in the Butcher tableau of the $s$-stage Gauss method (also known as $W$-transform [30]):

$$A = W X_s W^{-1}, \tag{34}$$

where matrix $X_s$ is defined at (32) and (see (28))

$$W = \begin{pmatrix} P_0(c_1) & \dots & P_{s-1}(c_1) \\ \vdots & & \vdots \\ P_0(c_s) & \dots & P_{s-1}(c_s) \end{pmatrix} \equiv \mathscr{P}_s,$$

$P_j$ being the scaled Legendre polynomials satisfying (7), and $\{c_1, \dots, c_s\}$ the Gauss-Legendre abscissae in $[0,1]$.

It is easy to prove that the criterion (33) turns out to be always satisfied if we replace matrix $A$ in (34) by

$$\hat{A} = W\left(X_s + Y\right) W^{-1}, \quad \text{with} \quad Y^T = -Y. \tag{35}$$

In particular, we select the skew-symmetric matrix $Y$ in the form

$$Y = \alpha \left( e_2 e_1^T - e_1 e_2^T \right), \tag{36}$$

with $\alpha \in \mathbb{R}$, and $e_i \in \mathbb{R}^s$ the $i$th unit vector, $i = 1, 2$. Consequently, we obtain a family of symplectic methods depending on a real parameter $\alpha$. It can be shown that, under mild assumptions [15], at each step we can choose a specific value $\alpha$ satisfying

$$\alpha = O(h^{2(s-1)}) \tag{37}$$

such that the Hamiltonian is exactly preserved in the new approximation. Moreover, exploiting (37), one proves that the original order $2s$ of the underlying $s$-stage Gauss method is retained by the new method. Consequently, for any initial condition $y_0$ and step-size $h$ (smaller than a suitably small $h_0 > 0$), there exists a sequence of parameters $\{\alpha_n\}_{n \geq 0}$, such that both the Hamiltonian and any quadratic invariant of (1) are preserved along the numerical trajectory $y_n \equiv y_n(\alpha_n, h)$, $n \geq 1$.

**Example 1** *When $s = 2$, one obtains the fourth-order EQUIP variant of the 2-stage Gauss method depicted in Table 1. The 2-stage Gauss method is retrieved for $\alpha = 0$.*

**Example 2** *In the case $s = 3$, one obtains the sixth-order EQUIP variant of the 3-stage Gauss method depicted in Table 2. Also in this case, for $\alpha = 0$ one retrieves the original 3-stage Gauss method.*

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**TABLE 1.** Fourth-order EQUIP method with $s = 2$ stages.

| | | |
|---|---|---|
| $\frac{1}{2} - \frac{\sqrt{3}}{6}$ | $\frac{1}{4}$ | $\frac{1}{4} - \frac{\sqrt{3}}{6} - \alpha$ |
| $\frac{1}{2} + \frac{\sqrt{3}}{6}$ | $\frac{1}{4} + \frac{\sqrt{3}}{6} + \alpha$ | $\frac{1}{4}$ |
| | $\frac{1}{2}$ | $\frac{1}{2}$ |

**TABLE 2.** Sixth-order EQUIP method with $s = 3$ stages.

| | | | |
|---|---|---|---|
| $\frac{1}{2} - \frac{\sqrt{15}}{10}$ | $\frac{5}{36}$ | $\frac{2}{9} - \frac{\sqrt{15}}{15} - 4\alpha\frac{\sqrt{5}}{15}$ | $\frac{5}{36} - \frac{\sqrt{15}}{30} - \alpha\frac{\sqrt{5}}{3}$ |
| $\frac{1}{2}$ | $\frac{5}{36} + \frac{\sqrt{15}}{24} + \alpha\frac{\sqrt{5}}{6}$ | $\frac{2}{9}$ | $\frac{5}{36} - \frac{\sqrt{15}}{24} - \alpha\frac{\sqrt{5}}{6}$ |
| $\frac{1}{2} + \frac{\sqrt{15}}{10}$ | $\frac{5}{36} + \frac{\sqrt{15}}{30} + \alpha\frac{\sqrt{5}}{3}$ | $\frac{2}{9} + \frac{\sqrt{15}}{15} + 4\alpha\frac{\sqrt{5}}{15}$ | $\frac{5}{36}$ |
| | $\frac{5}{18}$ | $\frac{4}{9}$ | $\frac{5}{18}$ |

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