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Citation: *AIP Conf. Proc.* **1281**, 227 (2010); doi: 10.1063/1.3498430

View online: <http://dx.doi.org/10.1063/1.3498430>

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Energy and Quadratic Invariants Preserving Integrators of Gaussian Type¹

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Abstract. Recently, a whole class of energy-preserving integrators has been derived for the numerical solution of Hamiltonian problems [3, 2, 4]. In the mainstream of this research [6], we have defined a new family of symplectic integrators depending on a real parameter α [7]. For $\alpha = 0$, the corresponding method in the family becomes the classical Gauss collocation formula of order $2s$, where s denotes the number of the internal stages. For any given non-null α , the corresponding method remains symplectic and has order $2s - 2$: hence it may be interpreted as a $O(h^{2s-2})$ (symplectic) perturbation of the Gauss method. Under suitable assumptions, it can be shown that the parameter α may be properly tuned, at each step of the integration procedure, so as to guarantee energy conservation in the numerical solution. The resulting method shares the same order $2s$ as the generating Gauss formula, and is able to preserve both energy and quadratic invariants.

Keywords: Hamiltonian systems, collocation Runge-Kutta methods, symplectic integrators, energy-preserving methods.

PACS: 65P10, 65L05.

INTRODUCTION

When dealing with the numerical integration of canonical Hamiltonian systems in the form

$$\begin{cases} \dot{y} = J\nabla H(y) \equiv f(y), \\ y(t_0) = y_0 \in \mathbb{R}^{2m}, \end{cases} \quad J = \begin{pmatrix} 0 & I \\ -I & 0 \end{pmatrix} \in \mathbb{R}^{2m \times 2m}, \quad (1)$$

(I is the identity matrix of dimension m), two main lines of investigation may be traced in the current literature, having as objective the definition and the study of symplectic methods and energy-conserving methods, respectively. In fact, the symplecticity of the map and the conservation of the energy function are the most relevant features characterizing a Hamiltonian system.

From the very beginning of this research activity, high order symplectic formulae were already available within the class of Runge-Kutta methods [11, 24, 23], the Gauss collocation formulae being one noticeable example. One important implication of symplecticity of the discrete flow, for Gauss-Legendre methods, is the conservation of quadratic invariants. This circumstance makes the symplecticity property of the method particularly appealing in the numerical simulation of isolated mechanical systems in the form (1), since it provides a precise conservation of the total angular momentum during the time evolution of the state vector. As a further positive consequence, a symplectic method also conserves quadratic Hamiltonian functions (see the monographs [15, 20] for a thorough analysis of symplectic methods).

Conversely, if one excludes the quadratic case, energy-conserving methods were initially not known within classical integration methods. The unsuccessful attempts to derive energy-preserving Runge-Kutta methods for polynomial Hamiltonians, culminated in the general feeling that such methods could not even exist (see [19] and [9]). 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 whatever the choice of the stepsize of integration (see [13, 21]).

More recently, the conservation of energy has been approached by means of the definition of the *discrete line integral*, in a series of papers (such as [17, 18]), leading to the definition of *Hamiltonian Boundary Value Methods* (HBVMs) (see for example [3, 2, 4, 5, 1]). They are a class of methods able to preserve, in the discrete solution, poly-

¹ Work developed within the project “Numerical Methods and Software for Differential Equations”.

nomial Hamiltonians of arbitrarily high degree (and, hence, a *practical* conservation of any sufficiently differentiable Hamiltonian. Such methods admit a Runge-Kutta formulation which reveals their close relationship with classical collocation formulae [6]. An infinity extension of HBVMs has also been proposed in [5] and [14]. These limit methods may be interpreted as a generalization of the *averaged vector field method* defined in [22].

Attempts to incorporate both symplecticity and energy conservation into the numerical method will clash with two non-existence results. The first [12] 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, it states that

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 [10] 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.

Despite these discouraging results, in [7] a new class of symplectic integrators of arbitrarily high-order has been proposed which, under some mild assumptions (see the next section), may share both features, in the sense specified in the theorem below. We prefer the use of the term "integrator" rather than method since, strictly speaking, our integrator may select a different symplectic formula from one integration step to the next, in order to enforce the energy conservation property. In what follows, we sketch the main ideas behind this approach. For further generalizations, as well as for a number of numerical evidences, we refer to [7]. We will begin with introducing a family of one-step methods

$$y_1(\alpha, h) = \Phi_h(y_0, \alpha) \quad (2)$$

(h is the stepsize of integration), depending on a real parameter α , with the following specifics:

1. for any fixed choice of $\alpha \neq 0$, the corresponding method is a symplectic Runge-Kutta method with s stages and of order $2s - 2$, which exactly conserves all quadratic invariants;
2. for $\alpha = 0$ one gets the Gauss collocation method (of order $2s$);
3. for any choice of y_0 and in a given range of the stepsize h , there exists a value of the parameter, say α_0 , depending on y_0 and h , such that $H(y_1(\alpha_0, h)) = H(y_0)$ (energy conservation).

The parametric method (2) realizes a symplectic perturbation of the Gauss method of size $O(h^{2s-2})$. Under suitable assumptions, as the parameter α ranges in a small interval centered at zero, the value of the numerical Hamiltonian function $H(y_1)$ will match $H(y(t_0 + h))$ thus leading to energy conservation. This result is formalized as follows:

Theorem 1 (Energy conservation) *Under suitable assumptions, there exists a real sequence $\{\alpha_k\}$ such that the numerical solution defined by $y_{k+1} = \Phi_h(y_k, \alpha_k)$, with y_0 defined in (1), satisfies $H(y_k) = H(y_0)$.*

One important remark is in order to clarify this statement and how it relates to the above non-existence results. Let us select the value of the parameter $\alpha = \alpha_0$, if any, in order to enforce the energy conservation between the two state vectors y_0 and y_1 , as indicated at item 3 above²: the map $y \mapsto \Phi_h(y, \alpha_0)$ is symplectic and, by definition, assures the energy conservation condition $H(y_1) = H(y_0)$. However, it is worth noticing that it would fail to provide a conservation of the Hamiltonian function if we changed the initial condition y_0 or the stepsize h . For example, in general for any $\hat{y}_0 \neq y_0$, we would obtain $H(\Phi_h(\hat{y}_0, \alpha_0)) \neq H(y_0)$: in this case we should change the value of the parameter α in order to recover the equality condition.³ Strictly speaking, the energy conservation property described in Theorem 1 weakens the standard energy conservation condition mentioned in the two non-existence results stated above and hence our methods are not meant to produce a counterexample of these statements.

² To avoid any misunderstanding, we emphasize that the value α_0 is now maintained constant, otherwise the map would fail to be symplectic.

³ More in general, the sequence $\{\hat{\alpha}_k\}$ that will satisfy Theorem 1 starting at \hat{y}_0 will differ from the sequence $\{\alpha_k\}$. Such sequences will be defined as the solution of the nonlinear system (7), as described in the next section.

DEFINITION OF THE METHODS

Let $\{c_1 < c_2 < \dots < c_s\}$ and $\{b_1, \dots, b_s\}$ be the abscissae and the weights of the Gauss-Legendre quadrature formula in the interval $[0, 1]$. We consider the Legendre polynomials $P_j(\tau)$ of degree $j - 1$, for $j = 1, \dots, s$, shifted and normalized in the interval $[0, 1]$ so that $\int_0^1 P_i(\tau)P_j(\tau)d\tau = \delta_{ij}$, for $i, j = 1, \dots, s$, (δ_{ij} is the Kronecker symbol), and the $s \times s$ matrix $\mathcal{P} = (P_j(c_i))$. Our starting point is the following well-known decomposition of the Butcher array A of the Gauss method of order $2s$ [16, pp. 77–84]:

$$A = \mathcal{P}X_s\mathcal{P}^{-1}, \quad (3)$$

where X_s is defined as

$$X_s = \begin{pmatrix} \frac{1}{2} & -\xi_1 & & & \\ \xi_1 & 0 & \ddots & & \\ & \ddots & \ddots & \ddots & \\ & & & \xi_{s-1} & -\xi_{s-1} \\ & & & & 0 \end{pmatrix}, \quad \text{with} \quad \xi_j = \frac{1}{2\sqrt{4j^2 - 1}}, \quad j = 1, \dots, s-1. \quad (4)$$

We now consider the matrix $X_s(\alpha)$ obtained by perturbing (4) as follows:

$$X_s(\alpha) = \begin{pmatrix} \frac{1}{2} & -\xi_1 & & & \\ \xi_1 & 0 & \ddots & & \\ & \ddots & \ddots & \ddots & \\ & & & \xi_{s-1} + \alpha & -(\xi_{s-1} + \alpha) \\ & & & & 0 \end{pmatrix} \equiv X_s + \alpha W_s, \quad (5)$$

where α is a real parameter, $W_s = (e_s e_{s-1}^T - e_{s-1} e_s^T)$, and, as usual, $e_j \in \mathbb{R}^s$ is the j th unit vector. The family of methods (2) we are interested in, is formally defined by the following tableau (see (3)–(5)):

$$\begin{array}{c|c} c_1 & \\ \vdots & \mathcal{A}(\alpha) \\ c_s & \end{array} \quad \text{with} \quad \mathcal{A}(\alpha) \equiv \mathcal{P}X_s(\alpha)\mathcal{P}^{-1} = A + \alpha\mathcal{P}W_s\mathcal{P}^{-1}. \quad (6)$$

$$| \quad b_1 \dots b_s$$

Therefore $A(0) = A$ and, moreover, the following result holds true [7].

Theorem 2 *For any fixed value of α , the Runge-Kutta method (6) is symmetric and symplectic. For $\alpha = 0$, the usual Gauss-Legendre method of order $2s$ is recovered. For any fixed $\alpha \neq 0$, a method of order $2s - 2$ is obtained.*

If we can choose $\alpha \equiv \alpha_0$ so that the energy-conservation property be satisfied, then, one obtains a (*symmetric*), *Energy and QUadratic Invariants Preserving (EQUIP) method*, as specified in Theorem 1, of Gaussian type. Indeed, the conservation of quadratic invariants easily follows from the structure of the matrix (5) defining the method. In conclusion, these methods will provide an exact conservation of all quadratic invariants, besides the Hamiltonian function. In more details, if we denote, as usual, $Y = (Y_1^T \dots Y_s^T)^T$ the vector of the stages, $e = (1, \dots, 1)^T \in \mathbb{R}^s$, and defining the error function $g(\alpha, h) = H(y_1(\alpha, h)) - H(y_0)$, the nonlinear system, in the unknowns Y_1, \dots, Y_s and α , that is to be solved at each step for getting energy conservation, reads, for the given stepsize h ,

$$\begin{cases} Y = e \otimes y_0 + h(\mathcal{A}(\alpha) \otimes I)F(Y), \\ g(\alpha, h) = 0. \end{cases} \quad (7)$$

Concerning the question about the existence of a solution of (7), we make the following assumptions:

- (\mathcal{A}_1) the function g is analytical in a rectangle $[-\bar{\alpha}, \bar{\alpha}] \times [-\bar{h}, \bar{h}]$ centered at the origin;
- (\mathcal{A}_2) let d be the order of the error in the Hamiltonian function associated with the Gauss method applied to the given Hamiltonian system (1) and the given state vector y_0 , that is:

$$g(0, h) = H(y_1(0, h)) - H(y_0) = c_0 h^d + O(h^{d+1}), \quad c_0 \neq 0.$$

Then, we assume that for, any fixed $\alpha \neq 0$ in a suitable neighborhood of the origin,

$$g(\alpha, h) = c(\alpha)h^{d-2} + O(h^{d-1}), \quad c(\alpha) \neq 0.$$

Remark 1 We observe that, excluding the case where the Hamiltonian $H(y)$ is quadratic (which would imply $g(\alpha, h) = 0$, for all α), the error in the numerical Hamiltonian function associated with the Gauss method is expected to behave as $O(h^{2s+1})$. Consequently, $d \geq 2s$.

The following result then holds true [7].

Theorem 3 Under the assumptions (\mathcal{A}_1) and (\mathcal{A}_2) , there exists a function $\alpha_0 = \alpha_0(h)$, defined in a neighborhood of the origin $(-h_0, h_0)$, such that:

$$(i) \ g(\alpha_0(h), h) = 0, \text{ for all } h \in (-h_0, h_0); \quad (ii) \ \alpha_0(h) = \text{const} \cdot h^2 + O(h^3).$$

The next result concerns the order of convergence of the method (7) (again, the proof can be found in [7]).

Theorem 4 Consider the parametric method (6) and suppose that the parameter α is actually a function of the stepsize h , according to what stated in Theorem 3. Then, the resulting method has order $2s$.

Numerical tests concerning the new EQUIP methods of Gaussian type can be found in [7] and in the companion paper [8].

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