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Recent Advances on Preserving Methods for Poisson Systems

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Abstract. We present and analyze energy-conserving methods for the numerical integration of IVPs of Poisson type systems. They are also able to preserve some Casimirs. Their derivation and analysis is done following the ideas of Hamiltonian BVMs (HBVMs) (see [3] and references therein). The proposed methods turn out to be equivalent to those recently derived in [8], giving therefore an alternative point of view that provides additional insight on the methods. Sufficient conditions that ensure the existence of a unique solution of the implicit equations defining the formulae are given. A study of the implementation of the methods is provided.

Keywords: Ordinary differential equations; one-step methods; Poisson problems; Hamiltonian Boundary Value Methods; energy-preserving methods; line integral methods.
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INTRODUCTION

In this paper we deal with the numerical solution of Initial Value Problems (IVPs) in ordinary differential systems that can be written in the gradient form

$$\dot{\boldsymbol{y}}(t) = \mathbf{f}(\boldsymbol{y}(t)) \equiv B(\boldsymbol{y}(t))\,\nabla H(\boldsymbol{y}(t)), \quad t \in [0,h], \qquad \boldsymbol{y}(0) = \boldsymbol{y}_0 \in \mathbb{R}^m, \tag{1}$$

where $B(\boldsymbol{y})$ is a skew-symmetric matrix and $H = H(\boldsymbol{y})$ a scalar function that will be called the Hamiltonian function. The differential system of (1) has the first integral $H(\boldsymbol{y}) = \text{const}$, and numerical methods that preserve this integral are usually called energy-preserving methods. Further, any scalar function $C = C(\boldsymbol{y})$ such that $\nabla C(\boldsymbol{y})^T\, B(\boldsymbol{y}) \equiv 0$ is also a first integral called a Casimir function. In this paper we study numerical methods that provide a polynomial approximation $\boldsymbol{u}(t) \simeq \boldsymbol{y}(t)$, $t \in [0,h]$, to the solution, preserving the energy, in the sense that $H(\boldsymbol{u}(h)) = H(\boldsymbol{u}(0))$, and eventually possible Casimirs of (1). In the special case when (1) is a canonical Hamiltonian system, the derivation of methods that preserve the energy has been the subject of an extensive research in the last years. Among them, we may mention the so called "averaged vector field" of Quispel and Mc Laren [13], generalized later by Hairer in [9]. In more details, [9] describes the limit formulae of a particular instance of *Hamiltonian BVMs*, as is shown in [5]. At the best of our knowledge, the first instance of energy-preserving Runge-Kutta methods for polynomial Hamiltonian systems was given by Iavernaro and Pace [10] and, as observed in [7], they can also be derived by the discretization of the *averaged vector field method* in [13]. HBVMs were formerly presented in [4] (see also [2] and [3] and references therein), as a generalization of the *s-Stage Trapezoidal Methods* [10] and of the energy-preserving methods for polynomial Hamiltonians derived in [11, 12]. For Poisson type systems, in a recent paper of Cohen and Hairer [8], which, in turn, generalize the formulae presented in [9], some energy-preserving methods are proposed. In this paper we introduce and analyze a class of methods which are energy preserving. Since they are defined by a set of implicit equations, sufficient conditions for the existence of a unique solution are given. The relation with formulae in [8] is stablished and special attention is paid to the implementation of the methods. Further details and the proofs of the results are given in [1].

THE ENERGY-PRESERVING FORMULAE

We denote by $\{P_j(\tau)\}_{j\geq 0}$ the Legendre orthonormal polynomials shifted to $[0,1]$. For all $h > 0$ and real continuous function $g(t)$, $t \in [0,h]$ the series expansion of $g(\tau h)$, $\tau \in [0,1]$, in terms of Legendre polynomials can be written as

$$g(\tau h) = \sum_{j\geq 0} \gamma_j(g)\, P_j(\tau), \quad \tau \in [0,1], \qquad \gamma_j(g) = \int_0^1 P_j(\tau)\, g(\tau h)\, d\tau, \tag{2}$$

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where the coefficient $\gamma_j(g)$ can be interpreted as the projections of $g(\tau h)$ on the jth Legendre polynomial. In the use of vector valued polynomials we will denote by $\Pi_r^m(t)$ the set of m-vector polynomials in t with degree $\leq r$.

Definition 1 *Let r be a positive integer and $c_i, i = 1,\ldots,r$, the Gauss nodes of $P_r(\tau)$. The polynomial approximation $\boldsymbol{u}(\tau h) \in \Pi_r^m(t)$, to the solution $\boldsymbol{y}(\tau h)$, $\tau \in [0,1]$, of (1) is defined by the $r+1$ (vector) conditions*

$$\boldsymbol{u}(0) = \boldsymbol{y}_0, \qquad \dot{\boldsymbol{u}}(c_i h) = B\left(\boldsymbol{u}(c_i h)\right) \sum_{j=0}^{r-1} P_j(c_i)\, \gamma_j\left(\nabla H(\boldsymbol{u})\right), \quad i = 1,\ldots,r. \tag{3}$$

Since $\boldsymbol{u}(\tau h)$ is defined by implicit equations in (3), our first concern is to give sufficient conditions to ensure the existence of a unique solution. The following result holds true:

Theorem 1 *Assume that, for a given $\rho > 0$ and for a given norm $\|\cdot\|$ in $\mathbb{R}^m$, the functions $B = B(\boldsymbol{y})$ and $H = H(\boldsymbol{y})$ are $\mathscr{C}^1(\mathscr{V}_0)$ and $\mathscr{C}^2(\mathscr{V}_0)$, respectively, where $\mathscr{V}_0 = \{\boldsymbol{y} \in \mathbb{R}^m; \|\boldsymbol{y} - \boldsymbol{y}_0\| \leq \rho\}$. Then, there exist $h_0 > 0$ such that the vector valued polynomial $\boldsymbol{u}(\tau h)$ satisfying (3) exists and is unique, for all $0 \leq h \leq h_0$.*

The next results give the preservation and accuracy properties of the methods.

Theorem 2 *The method proposed in (3) preserves the energy of (1), that is, $H(\boldsymbol{u}(h)) = H(\boldsymbol{u}(0))$.*

Theorem 3 *The method proposed in (3) preserves all Casimir functions that are polynomial functions of degree ≤ 2.*

Theorem 4 *The method proposed in (3) has order $2r$, that is, $\boldsymbol{y}(h) - \boldsymbol{u}(h) = O(h^{2r+1})$.*

Next, we show that the formulae (3) are actually those defined in [8], so that we have here provided an alternative proof of their properties, which relies on the use of the orthonormal Legendre basis, in place of the Lagrange basis $\{\lambda_i(\tau)\}$ defined at the abscissae $\{c_i\}$.

Lemma 1 *Let $\lambda_i(\tau)$, $i = 1,\ldots,r$, be the Lagrange polynomials with respect to the Gauss abscissae $c_1,\ldots,c_r$. Then*

$$\sum_{j=0}^{r-1} P_j(c_i) P_j(\tau) = \lambda_i(\tau)/b_i, \qquad i = 1,\ldots,r, \qquad b_i = \int_0^1 \lambda_i(\tau)\,\mathrm{d}\tau. \tag{4}$$

Consequently, one obtains that the conditions of (3) can be rewritten as

$$\dot{\boldsymbol{u}}(c_i h) = B(\boldsymbol{u}(c_i h)) \int_0^1 \frac{\lambda_i(\tau)}{b_i} \nabla H(\boldsymbol{u}(\tau h))\,\mathrm{d}\tau, \qquad i = 1,\ldots,r,$$

i.e., the formulae defined in [8]. However, the choice of the orthonormal Legendre basis, in addition to provide an alternative way to study the properties of the methods, will in turn make more intuitive (in our opinion) the analysis and the implementation of the numerical methods obtained after the approximation of $\gamma_j(\nabla H(\boldsymbol{u}))$ in (3).

DISCRETIZATION

Clearly, formulae (3) don't yet provide numerical methods. These will be obtained once the integrals defining $\gamma_j(\nabla H(\boldsymbol{u}))$ are conveniently approximated by means of a quadrature formula. We will approximate them by means of a quadrature with $k \geq r$ nodes $\{\hat{c}_\ell\}$ and weights $\{\hat{b}_\ell\}$. Obviously, a good choice is to use a Gaussian set of points, thus providing a quadrature of order $2k$ which we assume hereafter. In such a case, the solution will not be $\boldsymbol{u}(t)$ anymore but another polynomial $\boldsymbol{\omega}(t) \in \Pi_r^m(t)$, satisfying

$$\dot{\boldsymbol{\omega}}(c_i h) = B\left(\boldsymbol{\omega}(c_i h)\right) \sum_{j=0}^{r-1} P_j(c_i)\, \hat{\gamma}_j\left(\nabla H(\boldsymbol{\omega})\right), \quad i = 1,\ldots,r, \tag{5}$$

$$\hat{\gamma}_j(\nabla H(\boldsymbol{\omega})) \equiv \sum_{\ell=1}^{k} \hat{b}_\ell P_j(\hat{c}_\ell) \nabla H(\boldsymbol{\omega}(\hat{c}_\ell h)) = \gamma_j(\nabla H(\boldsymbol{\omega})) + O(h^{2k-j}), \qquad j = 0,\ldots,r-1. \tag{6}$$

Remark 1 *In the particular case where $H(\boldsymbol{y})$ is a polynomial of degree ν, by considering that $\boldsymbol{\omega}$ is a polynomial of degree r, one obtains that $\gamma_j = \hat{\gamma}_j$, $j = 0,\ldots,r-1$, provided that $\nu \leq 2k/r$. This provides a* practical conservation *for all suitably regular Hamiltonians, by choosing k large enough, assuming the integrals are approximated within machine precision.*

Since $\dot{\boldsymbol{\omega}}(ch)$ is a polynomial of degree r, let us set $\dot{\boldsymbol{\omega}}(ch) = \sum_{i=0}^{r-1} P_i(c)\,\hat{\Gamma}_i$. Defining

$$\mathscr{P} = \left(P_{j-1}(\hat{c}_i)\right),\ \hat{\mathscr{P}} = \left(P_{j-1}(\hat{c}_i)\right),\ \hat{\mathscr{I}} = \left(\int_0^{\hat{c}_i} P_{j-1}(x)\,\mathrm{d}x\right) \in \mathbb{R}^{k\times r},\ \hat{\Omega} = \mathrm{diag}(\hat{b}_1,\ldots,\hat{b}_k),$$
$$\hat{\mathbf{\Gamma}} = (\hat{\Gamma}_0^T,\ldots,\hat{\Gamma}_{r-1}^T)^T,\quad B(\boldsymbol{v}) = \mathrm{diag}(B(\boldsymbol{v}(c_1h)),\ldots,B(\boldsymbol{v}(c_rh))),\quad \Omega = \mathrm{diag}(b_1,\ldots,b_k),$$
$$e = (1,\ldots,1)^T \in \mathbb{R}^r,\qquad \hat{e} = (1,\ldots,1)^T \in \mathbb{R}^k,\qquad \mathscr{I} = \left(\int_0^{c_i} P_{j-1}(x)\,\mathrm{d}x\right) \in \mathbb{R}^{r\times r},$$

the discrete problem (5)-(6) can be written as

$$\hat{\mathbf{\Gamma}} = (\mathscr{P}^T\Omega\otimes I)\,B\left(e\otimes y_0 + h(\mathscr{I}\otimes I)\hat{\mathbf{\Gamma}}\right)(\mathscr{P}\hat{\mathscr{P}}^T\hat{\Omega}\otimes I)\,\nabla H\left(\hat{e}\otimes y_0 + h(\hat{\mathscr{I}}\otimes I)\hat{\mathbf{\Gamma}}\right), \tag{7}$$

which has block size r, *independently of* k. Once (7) has been solved, the new approximation is given by

$$\boldsymbol{y}_1 = \boldsymbol{y}_0 + \sum_{j=0}^{r-1}\hat{\Gamma}_j\int_0^1 P_j(\sigma)\,\mathrm{d}\sigma = \boldsymbol{y}_0 + \hat{\Gamma}_0. \tag{8}$$

The next results extend to the discrete setting the results of Theorem 2 and Theorem 4.

Theorem 5 *For all $k \geq r$, one has $\boldsymbol{y}(h) - \boldsymbol{\omega}(h) = O(h^{2r+1})$.*

Theorem 6 *For all $k \geq r$, $H(\boldsymbol{\omega}(h)) - H(\boldsymbol{y}_0) = O(h^{2k+1})$. In addition, if $H(\boldsymbol{y})$ is a polynomial of degree $\nu \leq 2k/r$, then $H(\boldsymbol{\omega}(h)) = H(\boldsymbol{y}_0)$.*

On the other hand, it can be readily proved that the result of Theorem 3 continues to be valid after the discretization.

NUMERICAL TESTS

We consider the Poisson problem defined as follows:

$$B(\boldsymbol{y}) = \begin{pmatrix} 0 & c_3y_3 & -c_2y_2 \\ -c_3y_3 & 0 & c_1y_1 \\ c_2y_2 & -c_1y_1 & 0 \end{pmatrix},\qquad H(\boldsymbol{y}) = y_1^{12} + \frac{1}{2}\left[(y_2-y_3)^2 + (y_1-y_3)^2\right], \tag{9}$$

with $c_1 = 1, c_2 = 5, c_3 = -4$. The solution started at $(1,1,1)^T$ turns out to be periodic with period $T \approx 0.53102669598427$. The problem admits also the quadratic Casimir $C(\boldsymbol{y}) = (c_1y_1^2 + c_2y_2^2 + c_3y_3^2)/2$. We use the methods derived by formula (3) with $r = 2$, by considering $k = 12$ Gauss points for the numerical quadrature approximating the integrals. Consequently, the quadrature turns out to be exact for this polynomial Hamiltonian of degree $\nu = 12$, so that the method is energy conserving. Moreover, the quadratic Casimir turns out to be conserved. In the practice, we obtain a method closely related to the HBVM(12,2) method. In Table 1, we list the errors after one period by using the 2-stages Gauss method, and the (12,2) conservative variant (i.e., the method defined by (5)-(6) with $k = 12$ and $r = 2$). As one can see, the order four of the methods is numerically confirmed. Moreover, the error for the conserving method is smaller than that for the Gauss method, which turns out to preserve only the Casimir. This fact is further confirmed by considering a longer time interval, where the conserving method exibits a linear error growth, whereas the Gauss method has a quadratic error growth (along with a drift in the Hamiltonian), as is shown in Figure 1. We observe that the linear growth of the error with the (12,2) conserving method (which, actually, preserves two invariants of the problem), confirms the analysis in [6].

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TABLE 1. Problem (9), error after one period for the 2-stages Gauss method (e_G) and for the (12,2) conservative variant (e_{CV}), when using a stepsize $h = T/n$, along with the estimated order of convergence.

n	e_{CV}	p	e_G	p
20	1.287e-02	—	6.556e-01	—
40	2.124e-03	2.60	4.509e-02	3.86
60	4.589e-04	3.78	1.331e-02	3.01
80	1.510e-04	3.86	4.298e-03	3.93
100	6.300e-05	3.92	1.796e-03	3.91
120	3.068e-05	3.95	8.751e-04	3.94

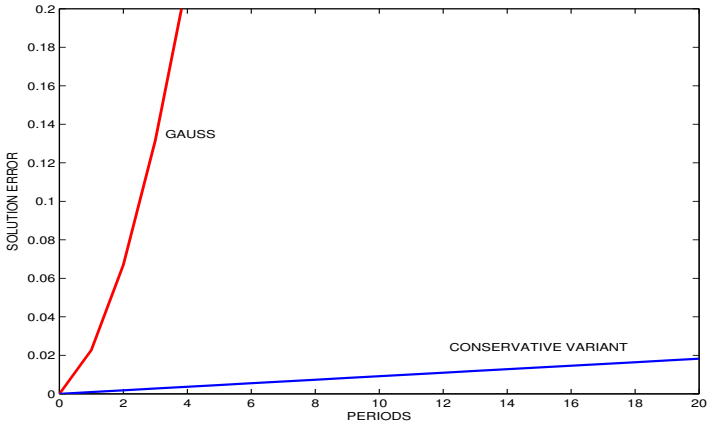

FIGURE 1. Problem (9), error in the computed solution by using the 2-stages Gauss method and the (12,2) conservative variant with a constant stepsize $h = T/50$.

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