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Modified Line Integral Methods for Conservative Problems with Multiple Invariants

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Abstract. In this paper we define a class of modified line integral methods, which are a suitable modification of energy conserving methods in the HBVMs class, able to cope with conservative problems possessing multiple invariants. The analysis of the methods is sketched, along with some numerical tests.

INTRODUCTION

Much attention has been devoted, in the last years, to the numerical solution of conservative problems (i.e., problems admitting constants of motion), with particular emphasis on Hamiltonian problems, which are in the form

$$y' = J\nabla H(y) \equiv f(y), \qquad y(0) = y_0 \in \mathbb{R}^{2m}, \tag{1}$$

with J a skew-symmetric matrix and H the Hamiltonian function of the problem, sometimes called the *energy*. Recently, the class of energy-conserving methods, called *Hamiltonian Boundary Value Methods (HBVMs)*, has been proposed [4, 5, 6, 7, 8]. Such methods, which are based on the concept of *discrete line integral*, provide a polynomial approximation, for $t \in [0, h]$, obtained by a local Fourier expansion of the right-hand side of the problem, along the orthonormal polynomial basis given by the scaled and shifted Legendre polynomials $\{P_j\}_{j\geq 0}$: $P_j \in \Pi_j$, $\int_0^1 P_i(x)P_j(x)\mathrm{d}x = \delta_{ij}$, $\forall i,j \geq 0$, with δ_{ij} the Kronecker symbol. The polynomial approximation σ, in the interval $[0,1]$ is defined as [8]:

$$\sigma'(ch) = \sum_{j=0}^{s-1} P_j(c)\gamma_j(\sigma), \qquad c \in [0,1], \tag{2}$$

where (see Lemma 1 in [8])

$$\gamma_j(\sigma) = \int_0^1 P_j(\tau)f(\sigma(\tau h))\mathrm{d}\tau = O(h^j), \qquad j \geq 0.$$

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

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

Discretizing the involved integrals by using a Gauss-Legendre quadrature formula of order $2k$ (i.e., based at the k zeros of P_k), yields a HBVM(k,s) method. From the properties of Legendre polynomials, it follows that the approximation to $y(h)$ is given by $\sigma(h) = y_0 + h\gamma_0(\sigma)$. A HBVM$(k,s)$ admits a Runge-Kutta formulation [7] and, for all $k \geq s$, it satisfies the properties listed below [5, 8]:

- it is symmetric and has order $2s$ (when $k = s$ one retrieves the s-stage Gauss-Legendre collocation method);
- it is energy conserving for all polynomial Hamiltonians of degree not larger than $2k/s$;
- for general, suitably regular Hamiltonians, one has $H(\sigma(h)) - H(\sigma(0)) = O(h^{2k+1})$.

From the last point, one infers that (an at least practical) energy conservation can be always gained by choosing k suitably large, also considering that the computational cost essentially depends on s, rather than on k [6, 2]. Such methods have been generalized along several directions (see, e.g., [1, 3, 7, 10]), in order to cope with general conservative problems, and/or Hamiltonian problems with multiple invariants. We here sketch a further generalization, aimed at solving conservative problems with multiple invariants (a more detailed analysis will be provided elsewhere). For sake of brevity, we shall consider problem (1), even though the new methods also work for general conservative problems.

MODIFIED LINE INTEGRAL METHODS

Assume that $G : \mathbb{R}^{2m} \to \mathbb{R}^{\nu}$, with $\nu < 2m$, is a set of (suitably regular) functionally independent invariants (also including the Hamiltonian). In order to have their conservation, let us define

$$\Phi_j(\sigma) = \int_0^1 P_j(\tau) \nabla G(\sigma(\tau h)) d\tau = O(h^j), \qquad j \geq 0,$$

where the last equality follows from Lemma 1 in [8], so that $\nabla G(\sigma(ch)) = \sum_{j \geq 0} P_j(c) \Phi_j(\sigma)$, $c \in [0,1]$, and

$$G(\sigma(h)) - G(y_0) = h \int_0^1 \nabla G(\sigma(\tau h))^\top \sigma'(\tau h) d\tau = h \sum_{j=0}^{s-1} \Phi_j(\sigma)^\top \gamma_j(\sigma).$$

Considering that (see Lemma 1 in [3])

$$\sum_{j=0}^{s-1} \Phi_j(\sigma)^\top \gamma_j(\sigma) = -\sum_{j \geq s} \Phi_j(\sigma)^\top \gamma_j(\sigma) = O(h^{2s}),$$

let us look for a new polynomial approximation,

$$\hat{\sigma}'(ch) = (I + h^{2s}F)\sigma'(ch) \equiv (I + h^{2s}F) \sum_{j=0}^{s-1} P_j(c) \gamma_j(\sigma), \tag{3}$$

where matrix $F \in \mathbb{R}^{2m \times 2m}$ is to be determined by imposing the conservation of all invariants. Setting

$$y_1 \equiv \hat{\sigma}(h) = y_0 + h \int_0^1 \hat{\sigma}'(\tau h) d\tau \equiv \sigma(h) + h^{2s+1} F \gamma_0(\sigma) \equiv \sigma(h) + \hat{F} \gamma_0(\sigma), \tag{4}$$

one obtains

$$
\begin{aligned}
0 &= G(y_1) - G(y_0) = h \int_0^1 \nabla G(\hat{\sigma}(\tau h))^\top \hat{\sigma}'(\tau h) d\tau = h \int_0^1 \nabla G(\hat{\sigma}(\tau h))^\top (I + h^{2s}F) \sigma'(\tau h) d\tau \\
&= h \sum_{j=0}^{s-1} \Phi_j(\hat{\sigma})^\top (I + h^{2s}F) \gamma_j(\sigma) = h \sum_{j=0}^{s-1} \Phi_j(\hat{\sigma})^\top (I + h^{2s}F) \gamma_j(\sigma) \\
&= h \sum_{j=0}^{s-1} \Phi_j(\hat{\sigma})^\top \gamma_j(\sigma) + h^{2s+1} \sum_{j=0}^{s-1} \Phi_j(\hat{\sigma})^\top F \gamma_j(\sigma) \equiv -h^{2s+1} f + h^{2s+1} \sum_{j=0}^{s-1} \Phi_j(\hat{\sigma})^\top F \gamma_j(\sigma),
\end{aligned}
$$

with $f = O(1)$. Consequently, one has to solve the matrix equation $\sum_{j=0}^{s-1} \Phi_j(\hat{\sigma})^\top F \gamma_j(\sigma) = f$. By setting $x = \text{vec}(F)$ (i.e., the vector containing columns $1, \ldots, 2m$ of matrix F), the latter equation may be recast in tensor form as

$$\sum_{j=0}^{s-1} [\gamma_j(\sigma) \otimes \Phi_j(\hat{\sigma})]^\top x \equiv M_F x = f. \tag{5}$$

Considering that $M_F \in \mathbb{R}^{\nu \otimes (2m)^2}$, with $\nu < 2m$, the system turns out to be underdetermined. We observe that M_F (which has $O(1)$ entries) has full rank, for all sufficiently small stepsizes h, under the following assumption:

$$\text{rank}\,(\gamma_0(\sigma) \otimes \Phi_0(\sigma)) = \nu, \qquad \text{as} \qquad h \to 0. \tag{6}$$

One easily realizes that (6) trivially holds true, provided that $f(y_0) \neq 0$, since the invariants are assumed to be functionally independent. The following property then easily follows, by means of arguments similar to those used to prove Theorem 1 in [8].

Theorem 1 *Under assumption (6), $y_1 - y(h) = O(h^{2s+1})$, that is, the new approximation has still order 2s.*

Definition 1 *We name* modified HBVM(k,s) *(m-HBVM(k,s)) the method obtained from (2)÷(5), by approximating the involved integrals by means of the Gauss-Legendre formula of order 2k.*

We observe that equation (5) is actually nonlinear, since M_F depends on the unknown matrix F. Nevertheless, by observing that $\Phi_j(\hat{\sigma}) = (I + O(h^{2s}))\Phi_j(\sigma)$, one can resort to the simplified Newton method, resulting in the following (much cheaper) iteration (see (4)):

$$\text{Initialize}: \quad \hat{x}_0 = 0, \quad F_0 = O, \quad M = M_{F_0}, \quad y_1^0 = \sigma(h) \equiv y_0 + h\gamma_0(\sigma).$$

$$\text{Compute}: \quad M = U\Sigma V^\top, \text{ the reduced SVD factorization of matrix } M, \text{ and, then, } M^+ = V\Sigma^{-1}U^\top.$$

$$\text{For } \ell = 1, 2, \dots: \quad \text{compute} \quad \hat{x}_\ell = \hat{x}_{\ell-1} - M^+\left(G(y_1^{\ell-1}) - G(y_0)\right),$$

$$\text{set } \hat{F}_\ell \text{ such that } \text{vec}(\hat{F}_\ell) \equiv \hat{x}_\ell,$$

$$\text{define (see (4)) the new approximation } y_1^\ell = y_1^0 + \hat{F}_\ell \gamma_0(\sigma).$$

NUMERICAL EXAMPLES

We here report a few numerical tests on the Kepler problem [3], defined by the Hamiltonian

$$H(q_1, q_2, p_1, p_2) = \frac{1}{2}\left(p_1^2 + p_2^2\right) - \frac{1}{\sqrt{q_1^2 + q_2^2}}. \tag{7}$$

When starting at $q_1(0) = 1 - \varepsilon$, $q_2(0) = p_1(0) = 0$, $p_2(0) = \sqrt{\frac{1+\varepsilon}{1-\varepsilon}}$, with $\varepsilon \in (0,1)$, the solution is periodic, of period $T = 2\pi$, and is given by an ellipse with eccentricity ε in the (q_1, q_2)-plane. This problem admits two additional invariants, besides the Hamiltonian (7), i.e., the angular momentum,

$$M(q_1, q_2, p_1, p_2) = q_1 p_2 - q_2 p_1, \tag{8}$$

and the Laplace-Runge-Lenz (LRL) vector,

$$L(q_1, q_2, p_1, p_2) = q_2 p_1^2 - q_1 p_1 p_2 - \frac{q_2}{\sqrt{q_1^2 + q_2^2}}. \tag{9}$$

We solve this problem for $\varepsilon = 0.9$, by using a constant stepsize $h = \frac{2\pi}{160}$ over 100 periods, with the following methods:

- the symplectic 3-stage Gauss method (which preserves the angular momentum, since the invariant is quadratic);
- the (practically) energy-conserving HBVM(9,3) method;
- the modified version of this latter method, m-HBVM(9,3), aimed at preserving all the three invariants.

In Figure 1 we plot the (absolute) errors for the invariants (7), (8), and (9), respectively, thus confirming that:

a) the 3-stage Gauss method doesn't conserve the Hamiltonian H and the LRL vector L, while conserving the angular momentum M;
b) the HBVM(9,3) method doesn't conserve the angular momentum M and the LRL vector L, while (practically) conserving the Hamiltonian H;
c) the m-HBVM(9,3) method is able to conserve all the three invariants.

This, in turn, reflects in the phase-plots in Figure 2, showing that the m-HBVM(9,3) method is the one producing the best approximated solution (which is exactly an ellipse).
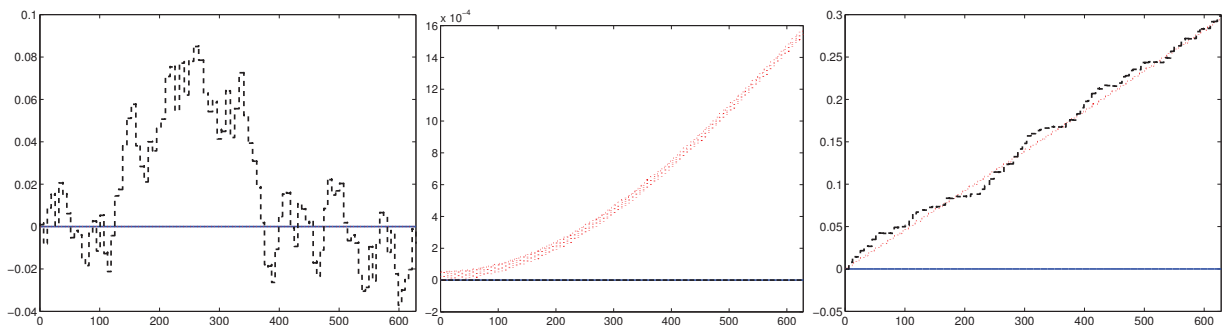
FIGURE 1. Absolute errors in the invariants: Hamiltonian (7) (left-plot); angular momentum (8) (middle-plot); LRL vector (9) (right-plot), by using the 3-stage Gauss method (dashed line), the HBVM(9,3) method (dotted line), and m-HBVM(9,3) method (solid line), with stepsize $h = 2\pi/160$, for solving the Kepler problem with $\varepsilon = 0.9$.
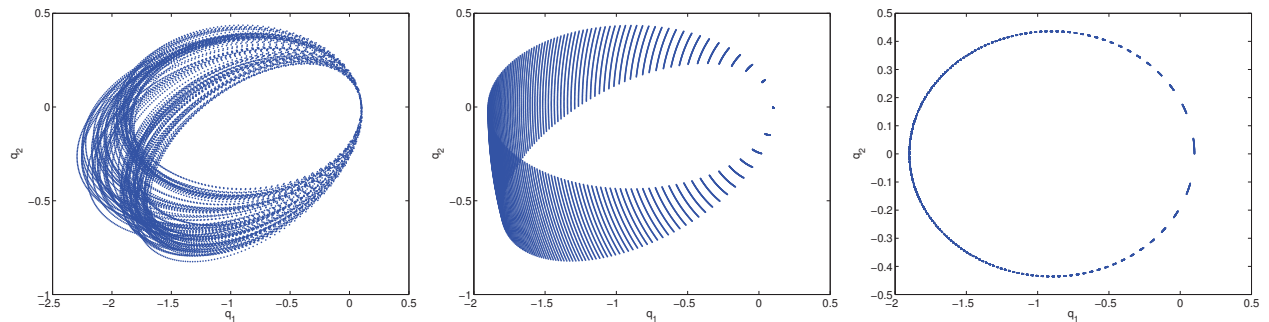
FIGURE 2. Obtained phase plots when solving the Kepler problem (with $\varepsilon = 0.9$) by using a stepsize $h = 2\pi/160$ with the following methods: 3-stage Gauss method (left-plot), HBVM(9,3) (middle-plot), and m-HBVM(9,3) (right-plot).

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