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Efficient Implementation of Geometric Integrators for Separable Hamiltonian Problems

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Abstract. We here investigate the efficient implementation of the energy-conserving methods named Hamiltonian Boundary Value Methods (HBVMs) recently introduced for the numerical solution of Hamiltonian problems. In this note, we describe an iterative procedure, based on a triangular splitting, for solving the generated discrete problems, when the problem at hand is separable.

Keywords: separable Hamiltonian problems, Energy-conserving Runge-Kutta methods, Hamiltonian Boundary Value Methods.
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MSC: 65P10; 65L05.

INTRODUCTION

Recently, the class of energy-conserving Runge-Kutta methods named *Hamiltonian Boundary Value Methods (HBVMs)* has been introduced for the efficient solution of Hamiltonian problems [8, 9, 10, 11, 12, 13]. Further generalization of such methods have been also devised [2, 4, 14], all essentially deriving from the original idea of *discrete line integral*, at first devised in [19, 20, 21]. For such methods, we propose an iterative procedure for solving the generated discrete problem, based on a suitable triangular splitting. The proposed approach follows the recent trend started in [6, 3]. Let then consider a separable Hamiltonian problem defined by the Hamiltonian $H(q,p) = \frac{1}{2}p^T p + U(q)$, that is,

$$q' = p, \qquad p' = -\nabla U(q), \qquad q(0) = q_0,\ p(0) = p_0 \in \mathbb{R}^m, \tag{1}$$

which we plan to assume to solve on the interval $[0,h]$. A HBVM(k,s) method, $k \geq s$, is a Runge-Kutta method defined by the Butcher tableau

$$\begin{array}{c|c} \mathbf{c} & \mathscr{I}_s \mathscr{P}_s^T \Omega \\ \hline & \mathbf{b}^T \end{array}, \qquad \mathbf{c} = (c_1,\ldots,c_k)^T, \qquad \mathbf{b} = (b_1,\ldots,b_k)^T,$$

with $\{c_\ell\}$ the k Gauss-Legendre abscissae on $[0,1]$, $\{b_\ell\}$ the corresponding weights, $\Omega = \mathrm{diag}(\mathbf{b})$, $\mathscr{I}_s = \left(\int_0^{c_i} P_{j-1}(x)\mathrm{d}x\right) \in \mathbb{R}^{k\times s}$, and, in general, $\mathscr{P}_r = \left(P_{j-1}(c_i)\right) \in \mathbb{R}^{k\times r}$, with $\{P_j\}_{j\geq 0}$ the Legendre polynomials orthonormal on [0,1]. Moreover, it is well-known that

$$\mathscr{I}_s = \mathscr{P}_{s+1}\hat{X}_s \equiv \mathscr{P}_{s+1}\left(\begin{array}{cccc} \frac{1}{2} & -\xi_1 & & \\ \xi_1 & 0 & \ddots & \\ & \ddots & \ddots & -\xi_{s-1} \\ & & \xi_{s-1} & 0 \\ \hline & & & \xi_s \end{array}\right) \equiv \left(\begin{array}{c} X_s \\ \hline 0\ldots 0\,\xi_s \end{array}\right), \quad \xi_j = (2\sqrt{4j^2-1})^{-1}, \quad j = 1,\ldots,s.$$

In particular, when $k = s$ one retrieves the usual s-stage Gauss method [10]. The following discrete problem then provides $O(h^{2s+1})$ approximations $q_1 = q_0 + h\mathbf{b}^T \otimes I_m P \approx q(h)$ and $p_1 = p_0 - h\mathbf{b}^T \otimes I_m \nabla U(Q) \approx p(h)$ [10, 12, 13],

$$Q = \mathbf{e}\otimes q_0 + h\mathscr{I}_s\mathscr{P}_s^T\Omega\otimes I_m P, \qquad P = \mathbf{e}\otimes p_0 - h\mathscr{I}_s\mathscr{P}_s^T\Omega\otimes I_m \nabla U(Q),$$

where $Q = (Q_1,\ldots,Q_k)^T$ and $P = (P_1,\ldots,P_k)^T$ are the stage vectors, $\mathbf{e} = (1,\ldots,1)^T \in \mathbb{R}^k$, and $\nabla U(Q) = (\nabla U(Q_1)^T,\ldots,\nabla U(Q_s)^T)^T$. Subsitution of the second equation into the first one, then gives, by considering that $\mathscr{I}_s\mathscr{P}_s^T\Omega\mathbf{e} = \mathbf{c}$ and $\mathscr{P}_s^T\Omega\mathscr{I}_s = X_s$,

$$Q = \mathbf{e}\otimes q_0 + h\mathbf{c}\otimes p_0 - h^2\mathscr{P}_{s+1}\hat{X}_s X_s \mathscr{P}_s^T\Omega\otimes I_m \nabla U(Q). \tag{2}$$

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TABLE 1. Auxiliary abscissae and diagonal entry of the matrix L, for $s = 2,3,4,5,6$.

$s=2$
$\hat{c}_1 = 0.3$
$\hat{c}_2 = 1$
$d_2 = 1/12$

$s=3$
$\hat{c}_1 = 0.18446492877530573726555810304564677 8$
$\hat{c}_2 = 0.35520661996767033759212466375803047 3$
$\hat{c}_3 = 0.11$
$d_3 = 0.04110353457217450169152685538590981 74$

$s=4$
$\hat{c}_1 = 0.12142636015430210954957371005350384 2$
$\hat{c}_2 = 0.32198301530914653476702551837153804 2$
$\hat{c}_3 = 0.55674665195682173785305626042539428 7$
$\hat{c}_4 = 0.0669$
$d_4 = 0.02439750182371332948385961590600250 47$

$s=5$
$\hat{c}_1 = 0.11202106164348446896744720787816595 1$
$\hat{c}_2 = 0.25064231874793011681838658566013556 9$
$\hat{c}_3 = 0.46853006043202850973016467340974264 9$
$\hat{c}_4 = 0.54958542438821906192671029493277414 4$
$\hat{c}_5 = 0.8432$
$d_5 = 0.01613493741827826427253049380882892 56$

$s=6$
$\hat{c}_1 = 0.02483107785625881510376290890541864 00$
$\hat{c}_2 = 0.08109274674555915561364300718008598 19$
$\hat{c}_3 = 0.16484216983630074562153162737911049 4$
$\hat{c}_4 = 0.28647397258281217890645429511984607 7$
$\hat{c}_5 = 0.82225293029450966363674314200439354 2$
$\hat{c}_6 = 0.43621$
$d_6 = 0.01145509013432089422202647128222134 70$

This problem has (block) dimension k, which may be significantly larger than s [10, 11, 13]. In order to recover a problem of (block) dimension s, independently of k, we set $\boldsymbol{\gamma} = \mathscr{P}_s^T \Omega \otimes I_m \nabla U(Q)$, thus resulting in the following discrete problem, obtained by substituting (2) in such an equation:

$$F(\boldsymbol{\gamma}) \equiv \boldsymbol{\gamma} - \mathscr{P}_s^T \Omega \otimes I_m \nabla U \left(\mathbf{e} \otimes q_0 + h\mathbf{c} \otimes p_0 - h^2 \mathscr{P}_{s+1} \hat{X}_s X_s \otimes I_m \boldsymbol{\gamma} \right) = \mathbf{0}.$$

Application of the simplified Newton method for its solution, then gives the following iteration, by taking into account that $\mathscr{P}_s^T \Omega \mathscr{P}_{s+1} \hat{X}_s X_s = [I_s \ \mathbf{0}] \hat{X}_s X_s = X_s^2$, and setting I the identity of dimension sm:

$$\text{Solve } \left[I + h^2 X_s^2 \otimes \nabla^2 U(q_0) \right] \Delta^j = -F(\boldsymbol{\gamma}^j), \qquad \text{then set } \boldsymbol{\gamma}^{j+1} = \boldsymbol{\gamma}^j + \Delta^j, \qquad j = 0,1,\ldots. \tag{3}$$

The efficient (possibly approximate) solution of the first linear system in (3) will be our main concern.

MODIFIED TRIANGULAR SPLITTING

Instead of solving the original linear system in (3), which would require the factorization of a matrix of dimension sm, we consider the following equivalent linear system,

$$\left[I + h^2 A_s \otimes \nabla^2 U(q_0) \right] \hat{\Delta}^j = \boldsymbol{\eta}_j,$$

where

$$A_s = \hat{\mathscr{P}}_s X_s^2 \hat{\mathscr{P}}_s^{-1}, \qquad \hat{\mathscr{P}}_s = \left(P_{j-1}(\hat{c}_i) \right) \in \mathbb{R}^{s \times s}, \qquad \hat{\Delta}_j = \hat{\mathscr{P}}_s \otimes I_m \Delta_j, \qquad \boldsymbol{\eta}_j = -\hat{\mathscr{P}}_s \otimes I_m F(\boldsymbol{\gamma}^j),$$

for a suitable choice of the set of *s auxiliary abscissae* $\hat{c}_1, \ldots, \hat{c}_s$. In particular, by following the approach used in [6, 3] (see also [18, 1]), these latter abscissae are chosen in order to obtain a Crout factorization $A_s = L_s U_s$, with L_s lower triangular and U_s upper triangular with unit diagonal entries, such that L_s has constant diagonal entries, all of them equals to $d_s = \sqrt[s]{\det X_s^2}$. Following the approach in [3], this allows us to express the first $s-1$ auxiliary abscissae $\hat{c}_1, \ldots, \hat{c}_{s-1}$ as a function of the last one, $\hat{c}_s$. This latter abscissa, in turn, is chosen in order to optimize the convergence properties of the following *inner* iteration, coupled with the *outer* iteration (3),

$$\text{Solve } \left[I + h^2 L_s \otimes \nabla^2 U(q_0) \right] \hat{\Delta}^{j,\ell+1} = h^2 [L_s - A_s] \otimes \nabla^2 U(q_0) \, \hat{\Delta}^{j,\ell} + \boldsymbol{\eta}_j, \qquad \ell = 0,1,\ldots, \tag{4}$$

by (approximately) minimizing its *maximum amplification factor* ρ^* which, if not larger than 1, makes the iteration P-convergent, according to [7]. The advantage of using the *inner* iteration (4) is that the coefficient matrix is lower block triangular, with diagonal block entries all equals to

$$D_s = I_m + h^2 d_s \nabla^2 U(q_0) \in \mathbb{R}^{m \times m},$$

TABLE 2. Convergence parameters.

s	ρ^*	$\tilde{\rho}$	$\tilde{\rho}_\infty$	ρ_1^*
2	0.25	0.08333	12	0.25
3	0.3546	0.06256	4.3307	0.4294
4	0.4168	0.03192	1.2575	0.5623
5	0.4931	0.03665	0.8351	0.6338
6	0.7295	0.03087	2.5826	0.9250

which is a *symmetric* matrix having the same size as that of the continuous problem (1), independently of s. In Table 1, we list the computed optimal auxiliary nodes, for $s = 2,\ldots,6$, along with the corresponding diagonal entry d_s, with 36 significant digits: one may see that the auxiliary nodes are all distinct and in the interval $[0,1]$. Their order (which is not commutative in the definition of matrix $\hat{\mathscr{P}}_s$) is the increasing one except, possibly, for last auxiliary abscissa, $\hat{c}_s$, which may not always be the largest one. According to the analysis in [7], a linear convergence analysis of the iteration (4) is obtained by considering the scalar problem $y'' = -\mu^2 y$, with $\mu \in \mathbb{R}$. By setting $x = h\mu \in \mathbb{R}$, one then obtains that the iteration matrix is given by

$$M(x^2) = x^2(I_s + x^2 L_s)^{-1} L_s (I_s - U_s),$$

whose spectral radius will be denoted by $\rho(x^2)$. Clearly, the iteration will be convergent if and only if $\rho(x^2) < 1$. We observe that $\rho(x^2) \to 0$, as $x \to \infty$. The *maximum amplification factor* [7] of the iteration is then defined as $\rho^* = \max_{x\geq 0} \rho(x^2)$. Moreover, according to the analysis in [7], one has $\rho(x^2) \approx \tilde{\rho} x^2$, for $x \approx 0$, and $\rho(x^2) \simeq \tilde{\rho}_\infty |x|^{-2/(s-1)}$, for $|x| \gg 1$. Clearly, the smaller the parameters ρ^*, $\tilde{\rho}$, and $\tilde{\rho}_\infty$, the better the iteration properties. In particular, the most important one is ρ^* which, if not larger than 1, makes the iteration P-convergent and, therefore, L-convergent (see [7] for full details). In Table 2 we list the convergence factors for the iteration (4). For sake of comparisons, in the last column we list the maximum amplification factor obtained by setting $\hat{c}_s = 1$ (denoted by ρ_1^*), as is done in [6]: the improvement by appropriately choosing the last auxiliary abscissa is evident, by comparing the last column in the table with the second one, containing the maximum amplification factor obtained by choosing $\hat{c}_s$ according to Table 1.

NUMERICAL TESTS

For assessing the effectiveness of the proposed iteration, we consider a problem for which the traditional fixed-point iteration may be not always effective, i.e., the Fermi-Pasta-Ulam problem, which is defined by the following Hamiltonian [17, page 21]:

$$H(q,p) = \frac{1}{2}\sum_{i=1}^{m}(p_{2i-1}^2 + p_{2i}^2) + \frac{\omega^2}{4}\frac{1}{2}\sum_{i=1}^{m}(q_{2i} - q_{2i-1})^2 + \sum_{i=0}^{m}(q_{2i+1} - q_{2i})^2, \qquad (q_0 = q_{2m+1} = 0).$$

Indeed, such a problem is an example of *stiff oscillatory* problem. We solve it with $\omega = 100$, $m = 3$, integration interval [0,10], and initial condition $q^0 = (0\ 1\ 2\ 3\ 4\ 5)^T/10$, $p^0 = (0\ 0\ 0\ 0\ 0\ 0)^T$, by using the following 4-th order methods: HBVM(4,2), which is energy-conserving, in such a case, and HBVM(2,2), i.e., the 2-stage Gauss method [10], which is symplectic but not energy conserving. Table 3 contains the computational costs, in terms of total iterations, required when using a constant stepsize $h = 2^{-i}10^{-1}$, $i = 0,\ldots,6$. For both methods we used the following iterative procedures for solving the generated discrete problems: the fixed-point iteration; the iterative procedure here described; the blended iteration, for special second order problems, as described in [11] (see also [15, 16]). Moreover, for the triangular splitting here described, we used either ν iterations (splitting-ν column in Table 3) in (4), where ν is the least value of iterations minimizing the total number of *outer* iterations (3) (ν is listed in the corresponding column), or we fixed $\nu = 2$ inner iterations (splitting-2 column in Table 3) since, in so doing, one *outer-inner* iteration (3)-(4) and one blended iteration as described in [11] have a comparable cost. From the obtained results, it follows that the outer-inner iteration, based on the modified triangular splitting here proposed, is the most effective one, among those considered, especially for coarser stepsizes (**** in Table 3 means that the iteration doesn't converge). We also observe that the number of iterations needed for solving the discrete problem, whichever the iterative method considered, is approximately independent of k, for a HBVM(k,s) method, but only depends on s. This fact has been systematically observed for such methods (see, e.g., [8, 10, 11, 12]) and is indeed confirmed also in the present case,

TABLE 3. Fermi-Pasta-Ulam problem: total number of iterations required by the HBVM(4,2) (left) and the 2-stage Gauss (right) methods, both used with stepsize $h = 2^{-i}10^{-1}$. The asterisks means that the iteration doesn't converge.

i	fixed-pt. iteration	splitting-ν iteration	ν	splitting-2 iteration	blended iteration
0	****	593	5	900	1592
1	****	1004	7	2550	4720
2	20622	1885	9	4784	9357
3	13506	3200	5	6384	12156
4	16178	5756	6	9364	15947
5	24374	9600	3	12800	24206
6	38229	19200	3	24889	38238

i	fixed-pt. iteration	splitting-ν iteration	ν	splitting-2 iteration	blended iteration
0	****	589	5	898	1585
1	****	1000	7	2531	4686
2	20453	1826	9	4776	9203
3	13468	3200	5	6376	11933
4	16000	5435	6	9205	15925
5	23756	9600	3	12800	23401
6	38100	19200	3	24405	38177

where we have considered the HBVM$(k,2)$ methods with $k = 4$ (energy-conserving) and $k = 2$ (2-stage symplectic Gauss method).

REFERENCES

1. P. Amodio, L. Brugnano. A Note on the Efficient Implementation of Implicit Methods for ODEs. *Journal of Computational and Applied Mathematics* **87** (1997) 1–9.
2. L. Brugnano, M. Calvo, J.I. Montijano, L. Ràndez. Energy preserving methods for Poisson systems. *J. Comput. Appl. Math.* **236** (2012) 3890–3904.
3. L. Brugnano, G. Frasca Caccia, F. Iavernaro. Efficient implementation of Gauss collocation and Hamiltonian Boundary Value Methods, 2013 *(submitted)*. `arXiv:1304.0974`
4. L. Brugnano, F. Iavernaro. Line Integral Methods which preserve all invariants of conservative problems. *J. Comput. Appl. Math.* **236** (2012) 3905–3919.
5. L. Brugnano, F. Iavernaro. Recent Advances in the Numerical Solution of Conservative Problems. *AIP Conf. Proc.* **1493** (2012) 175–182.
6. L. Brugnano, F. Iavernaro, C. Magherini. Efficient implementation of Radau collocation methods, 2012 *(submitted)*. `arXiv:1302.1037`
7. L. Brugnano, C. Magherini. Recent Advances in Linear Analysis of Convergence for Splittings for Solving ODE problems. *Applied Numerical Mathematics* **59** (2009) 542–557.
8. L. Brugnano, F. Iavernaro, D. Trigiante. Analisys of Hamiltonian Boundary Value Methods (HBVMs) for the numerical solution of polynomial Hamiltonian dynamical systems. (2009) `arXiv:0909.5659v1`
9. L. Brugnano, F. Iavernaro, D. Trigiante. Hamiltonian BVMs (HBVMs): A family of "Drift Free" methods for integrating polynomial Hamiltonian problems. *AIP Conf. Proc.* **1168** (2009) 715–718.
10. L. Brugnano, F. Iavernaro, D. Trigiante. Hamiltonian Boundary Value Methods (Energy Preserving Discrete Line Methods). *JNAIAM J. Numer. Anal. Ind. Appl. Math.* **5**,1-2 (2010) 17–37.
11. L. Brugnano, F. Iavernaro, D. Trigiante. A note on the efficient implementation of Hamiltonian BVMs. *J. Comput. Appl. Math.* **236** (2011) 375–383.
12. L. Brugnano, F. Iavernaro, D. Trigiante. The lack of continuity and the role of infinite and infinitesimal in numerical methods for ODEs: the case of symplecticity. *Appl. Math. Comput.* **218** (2012) 8053–8063.
13. L. Brugnano, F. Iavernaro, D. Trigiante. A simple framework for the derivation and analysis of effective one-step methods for ODEs. *Appl. Math. Comput.* **218** (2012) 8475–8485.
14. L. Brugnano, F. Iavernaro, D. Trigiante. Energy and quadratic invariants preserving integrators based upon Gauss collocation formulae. *SIAM J. Numer. Anal.* **50**, No. 6 (2012) 2897–2916.
15. L. Brugnano, C. Magherini. Blended Implementation of Block Implicit Methods for ODEs. *Appl. Numer. Math.* **42** (2002) 29–45.
16. L. Brugnano, C. Magherini. Blended Implicit Methods for solving ODE and DAE problems, and their extension for second order problems. *Jour. Comput. Appl. Mathematics* **205** (2007) 777–790.
17. E. Hairer, C. Lubich, G. Wanner. *Geometric Numerical Integration, Second Edition*, Springer, Berlin, 2006.
18. P.J. van der Houwen, J.J.B. de Swart. Parallel linear system solvers for Runge-Kutta methods. *Adv. Comput. Math.* **7**, 1-2 (1997) 157–181.
19. F. Iavernaro, B. Pace. *s*-Stage trapezoidal methods for the conservation of Hamiltonian functions of polynomial type. *AIP Conf. Proc.* **936** (2007) 603–606.
20. F. Iavernaro, B. Pace. Conservative Block-Boundary Value Methods for the solution of polynomial Hamiltonian systems. *AIP Conf. Proc.* **1048** (2008) 888–891.
21. F. Iavernaro, D. Trigiante. High-order symmetric schemes for the energy conservation of polynomial Hamiltonian problems. *JNAIAM J. Numer. Anal. Ind. Appl. Math.* **4**,1-2 (2009) 87–101.