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Numerical Comparisons among Some Methods for Hamiltonian Problems

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We here report a few numerical tests comparing geometric integrators, of Runge-Kutta type, described by Butcher tableaus in the following form:

\[
\begin{pmatrix}
c_1 \\
c_2 \\
\vdots \\
c_s \\
\end{pmatrix}
\begin{bmatrix}
\mathcal{P} X_s(\alpha) \mathcal{P}^{-1} \\
\mathcal{P} \check{X}_s \mathcal{P}^T \Omega \\
\end{bmatrix}
\begin{pmatrix}
b_1 & \ldots & b_s \\
b_1 & \ldots & b_k \\
\end{pmatrix}
\]

where \( k \geq s \), \( \{c_1 < c_2 < \ldots < c_s\} \) and \( \{b_1, \ldots, b_k\} \) are the abscissae and the weights of the Gauss-Legendre quadrature formula in the interval \([0, 1], \ell = s, k, \)

\[
X_s(\alpha) = \left( \begin{array}{cccc}
\frac{1}{2} & -\xi_1 & & \\
\xi_1 & 0 & & \\
& \ddots & \ddots & \\
\xi_{s-1} + \alpha & & \ddots & -\xi_1 \\
\end{array} \right), \quad \check{X}_s = \left( \begin{array}{cccc}
\frac{1}{2} & -\xi_1 & & \\
\xi_1 & 0 & & \\
& \ddots & \ddots & \\
\xi_{s-1} & & \ddots & -\xi_1 \\
0 & & \ddots & 0 \\
0 & & \ddots & \xi_s \\
\end{array} \right), \quad \xi_j = \frac{1}{2\sqrt{(4j^2 - 1)}},
\]

\( \Omega = \text{diag}(b_1, \ldots, b_k) \) and, finally, by considering the Legendre polynomials \( P_j(\tau) \) of degree \( j - 1 \), for \( j \geq 1 \), shifted and normalized in the interval \([0, 1] \) so that \( \int_0^1 P_j(\tau) P_j(\tau) d\tau = \delta_{jj} \) (the Kronecker symbol), \( \mathcal{P} = (P_j(c_i)) \in \mathbb{R}^{s \times s} \), \( \mathcal{P}_k = (P_j(c_i)) \in \mathbb{R}^{k \times k+1} \). Method (1)-(a) reduces to the \( s \)-stage Gauss-Legendre method when \( \alpha = 0 \) (see, e.g., [10, pp. 77 ff.]). The same happens to method (1)-(b) when \( k = s \) [5, 6]. The \( s \)-stage Gauss-Legendre method is known to be a symplectic integrator of order \( 2s \), able to preserve quadratic invariants for Hamiltonian problems in canonical form [9]. On the other hand, under suitable mild assumptions [7] the parameter \( \alpha \) in (1)-(a) can be tuned, at each step, in order to obtain also the conservation of the Hamiltonian (see also [8]): let us denote such methods by EQUIP(s) (Energy and QUadratic Invariants Preserving) methods. Finally, the formulae (1)-(b) define the class of HBVM(\( k, s \)) methods [2, 3, 4, 5, 6], able to preserve polynomial Hamiltonian functions of degree \( \nu \), provided that \( k \geq (\nu s)/2 \) (obviously, \( \text{a practical conservation of energy is obtained, for all suitably regular Hamiltonian functions, provided that} \ k \text{ is large enough}. \) The order of all the above mentioned methods is \( 2s \). In the following we fix \( s = 3 \).

In Figures 1–3 we plot the errors (in the solution, in the Hamiltonian, and in the angular momentum, respectively) versus the (constant) stepsize used, for the GAUSS(3) (\( \equiv \) HBVM(3,3)), HBVM(4,3), HBVM(6,3), HBVM(9,3), HBVM(12,3), and EQUIP(3) methods applied to the Kepler problem [9, pp. 7–9], with eccentricity \( e = 0.6 \), over 1000 periods. As one can see (Figure 1), the order of all methods is confirmed to be 6, even though the error constants of HBV(k,3), \( k > 3 \), and EQUIP(3) methods turn out to be apparently the same, and approximately 40 times less than that of GAUSS(3) (\( \equiv \) HBVM(3,3)). The error in the Hamiltonian (Figure 2), as expected, decreases for HBVM(\( k, s \)) methods, as \( k \) is increased (with order \( 2k \) [4], until round-off errors prevail), and practical conservation is obtained for \( k \geq 9 \). EQUIP(3) clearly conserves, by its own definition, the Hamiltonian. Finally (Figure 3), the error in the angular momentum (which is a quadratic invariant) is negligible for GAUSS(3) and EQUIP(3) methods, and decreasing at the
same rate 6 (≡ 2s) with the stepsize, for HBVM\((k,3)\), \(k > 3\), methods. This is to be expected, since this error only depends on matrix \( \hat{X}_3 \) (see (1)-(b)), which is the same for all such methods.

To conclude, we report the numerical results, by using variable stepsize with a standard stepsize selection strategy \((tol = 10^{-8})\), for the GAUSS(3), HBVM(12,3), and EQUIP(3) methods applied to the Kepler problem, with eccentricity \(e = 0.99\), over 100 periods. All methods select stepsizes in the range \(10^{-4} \div 10^{0}\). As is well known [9] standard stepsize strategies don’t work well with symplectic methods, so that GAUSS(3), though preserving the angular momentum, exhibits a drift in the numerical Hamiltonian (see Figures 4 and 5). On the contrary, HBVM(12,3) practically conserves the Hamiltonian but exhibits a drift in the angular momentum (see Figures 6 and 7). At last, from Figure 8 we conclude that only EQUIP(3) preserves both the energy and the angular momentum, when a standard mesh selection strategy is used.

REFERENCES

FIGURE 3.

FIGURE 4.

FIGURE 5.
FIGURE 6.

FIGURE 7.

FIGURE 8.