# Numerical Comparisons among Some Methods for Hamiltonian Problems

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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:

$$\text{(a)}\quad \begin{array}{c|c} c_1 & \\ \vdots & \mathscr{P}X_s(\alpha)\mathscr{P}^{-1} \\ c_s & \\ \hline & b_1\ \ldots\ b_s \end{array} \qquad \text{(b)}\quad \begin{array}{c|c} c_1 & \\ \vdots & \mathscr{P}_k\hat{X}_s\mathscr{P}_k^T\Omega \\ c_k & \\ \hline & b_1\ \ldots\ b_k \end{array} \tag{1}$$

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

$$X_s(\alpha) = \begin{pmatrix} \frac{1}{2} & -\xi_1 & & \\ \xi_1 & 0 & \ddots & \\ & \ddots & \ddots & -(\xi_{s-1}+\alpha) \\ & & \xi_{s-1}+\alpha & 0 \end{pmatrix}, \quad \hat{X}_s = \begin{pmatrix} \frac{1}{2} & -\xi_1 & & & \\ \xi_1 & 0 & \ddots & & \\ & \ddots & \ddots & -\xi_{s-1} & \\ & & \xi_{s-1} & 0 & \\ & & & \xi_s & 0 \end{pmatrix}, \quad \xi_j = \frac{1}{2\sqrt{4j^2-1}},$$

$\Omega = \mathrm{diag}(b_1,\ldots,b_k)$ 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 $\int_0^1 P_i(\tau)P_j(\tau)\mathrm{d}\tau = \delta_{ij}$ (the Kronecker symbol), $\mathscr{P} = (P_j(c_i)) \in \mathbb{R}^{s\times s}$, $\mathscr{P}_k = (P_j(c_i)) \in \mathbb{R}^{k\times s+1}$. 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($s$) (*E*nergy and *QU*adratic *I*nvariants *P*reserving) 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, a *practical* conservation of energy is obtained, for all suitably regular Hamiltonian functions, provided that $k$ 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($k$,3) 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

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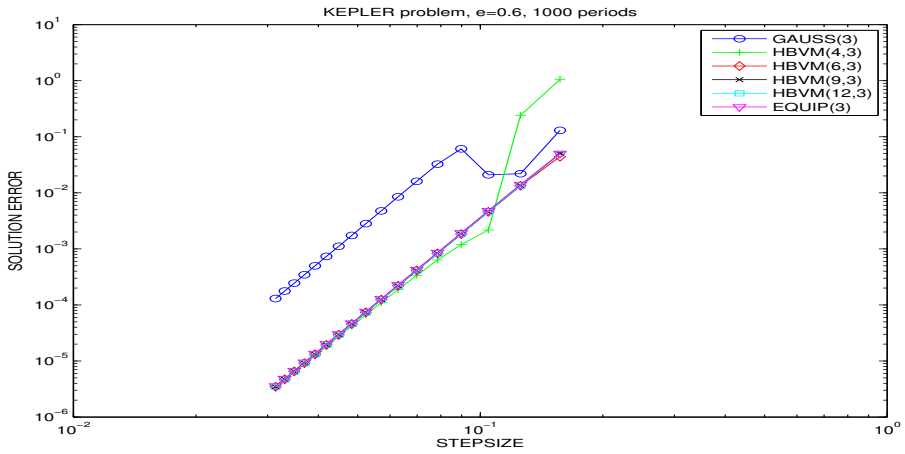


**FIGURE 1.**

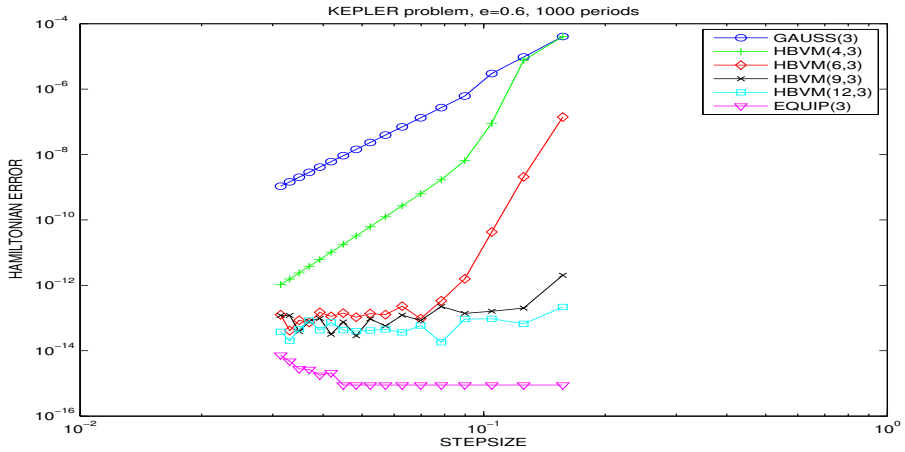


**FIGURE 2.**

same rate 6 ($\equiv 2s$) 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.

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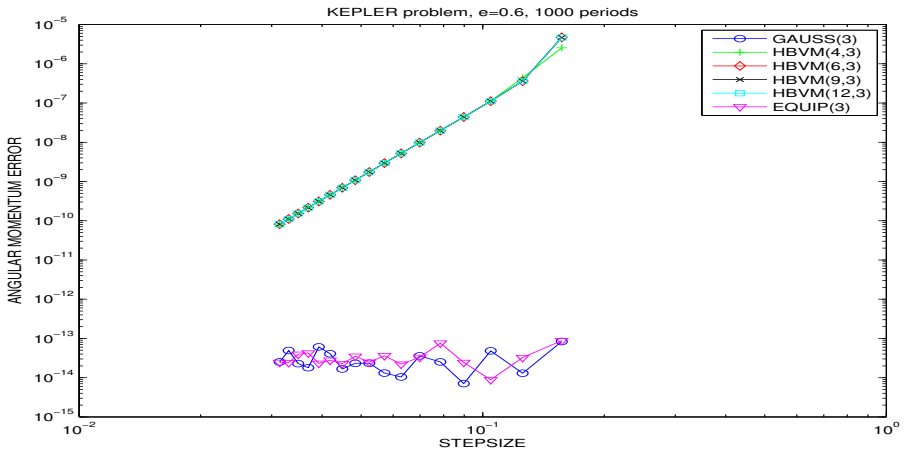
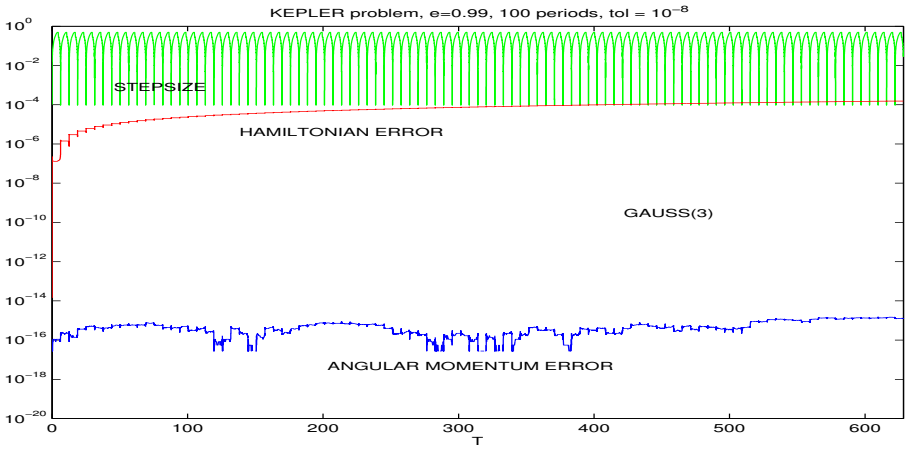



**FIGURE 3.**

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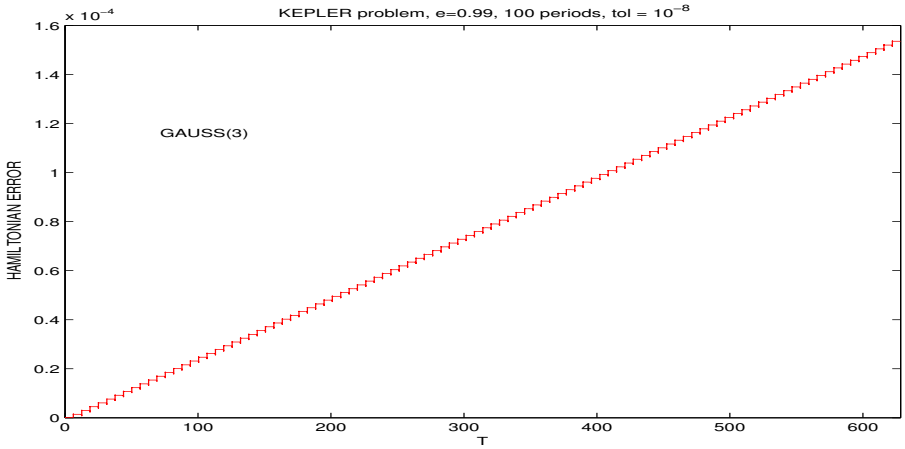


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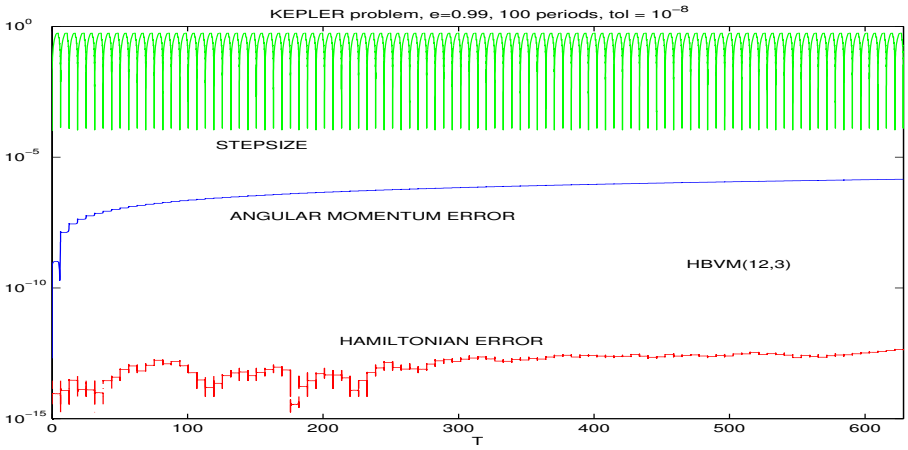


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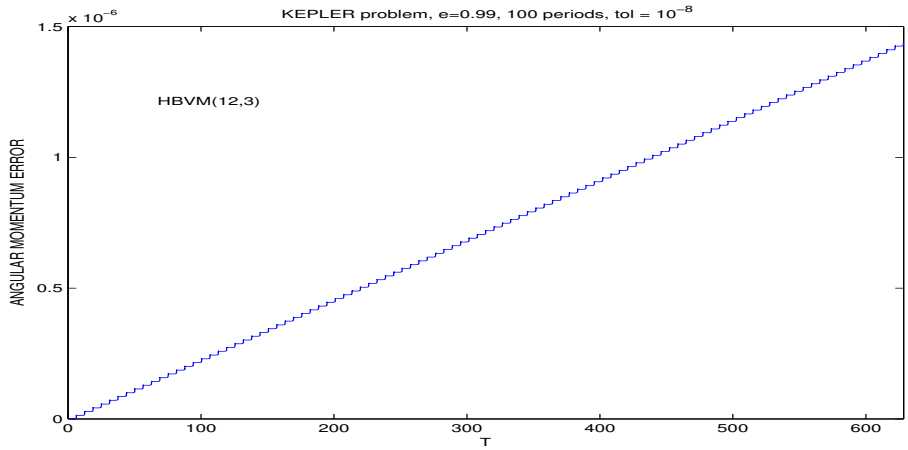


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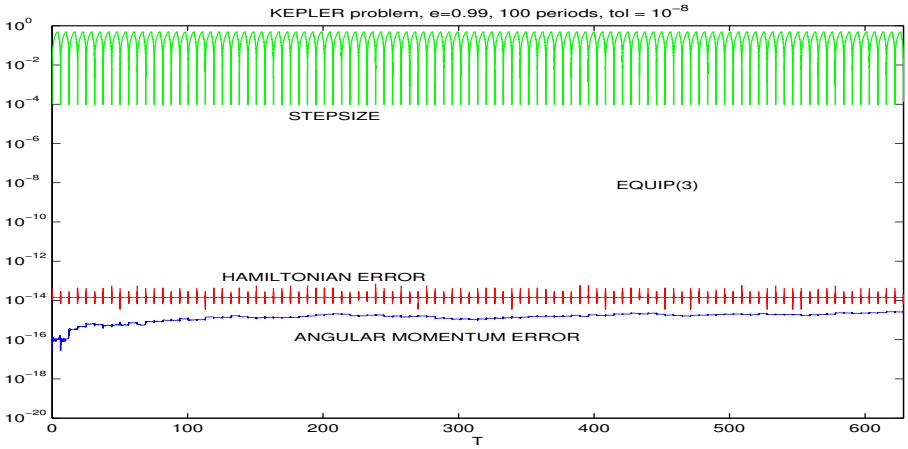


**FIGURE 8.**

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