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LACK OF DISSIPATIVITY IS NOT SYMPLECTICNESS *†

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Abstract.

We show that, when numerically integrating Hamiltonian problems, nondissipative numerical methods do not in general share the advantages possessed by symplectic integrators. Here a numerical method is called nondissipative if, when applied with a small stepsize to the test equation $dy/dt = i\lambda y$, λ real, has amplification factors of unit modulus. We construct a fourth order, nondissipative, explicit Runge-Kutta-Nyström procedure with small error constants. Numerical experiments show that this scheme does not perform efficiently in the numerical integration of Hamiltonian problems.

AMS subject classification: 65L05.

Key words: Hamiltonian problems, symplectic integrators, nondissipative methods, Runge-Kutta-Nyström procedures.

1 Introduction.

The purpose of this paper is to show that, when numerically integrating Hamiltonian problems, nondissipative numerical methods do not in general share the advantages possessed by symplectic integrators. Here a numerical method is called *nondissipative* if, when applied with a small stepsize to the test equation $dy/dt = i\lambda y$, λ real, has amplification factors of unit modulus.

We restrict our attention to Runge-Kutta-Nyström (RKN) methods (see e.g. [6], Section II.14) for systems of the special form

$$\frac{d\mathbf{p}}{dt} = \mathbf{f}(\mathbf{q}), \qquad \frac{d\mathbf{q}}{dt} = \mathbf{p}, \tag{1.1}$$

($\mathbf{p}$ and $\mathbf{q}$ are d-dimensional vectors) or equivalently to second order systems

$$\frac{d^2\mathbf{q}}{dt^2} = \mathbf{f}(\mathbf{q}).$$

The more general case where the second equation in (1.1) is replaced by $d\mathbf{q}/dt = M^{-1}\mathbf{p}$, with M a constant, invertible mass matrix might have also been catered for in what follows; only minor adjustments are required, cf. [13], Section 6.4.

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A step of length h with the RKN method of tableau

$$
\begin{array}{c|ccc}
\gamma_1 & \alpha_{11} & \cdots & \alpha_{1s} \\
\vdots & \vdots & \ddots & \vdots \\
\gamma_s & \alpha_{s1} & \cdots & \alpha_{ss} \\
\hline
 & \beta_1 & \cdots & \beta_s \\
\hline
 & b_1 & \cdots & b_s
\end{array}
\tag{1.2}
$$

is given by the formulae

$$
\begin{aligned}
\mathbf{p}^{n+1} &= \mathbf{p}^n + h\sum_{i=1}^{s} b_i \mathbf{f}(\mathbf{Q}_i), \\
\mathbf{q}^{n+1} &= \mathbf{q}^n + h\mathbf{p}^n + h^2\sum_{i=1}^{s} \beta_i \mathbf{f}(\mathbf{Q}_i),
\end{aligned}
$$

where $\mathbf{Q}_i$, $i = 1, \ldots, s$, are the stage vectors defined by

$$
\mathbf{Q}_i = \mathbf{q}^n + h\gamma_i \mathbf{p}^n + h^2 \sum_{j=1}^{s} \alpha_{ij} \mathbf{f}(\mathbf{Q}_j).
$$

As it is customary, we impose throughout the standard simplifying assumptions given by

$$
\beta_i = b_i(1 - \gamma_i), \quad i = 1, \ldots, s. \tag{1.3}
$$

In the particular instance of the scalar test problem given by the harmonic oscillator ($\lambda \neq 0$ is real)

$$
\frac{dq^2}{dt^2} = -\lambda^2 q,
$$

the application of an RKN method leads to a recursion

$$
\begin{bmatrix} p^{n+1} \\ q^{n+1} \end{bmatrix} = \begin{bmatrix} R_{11}(h^2\lambda^2) & h^{-1}R_{12}(h^2\lambda^2) \\ hR_{21}(h^2\lambda^2) & R_{22}(h^2\lambda^2) \end{bmatrix} \begin{bmatrix} p^n \\ q^n \end{bmatrix}, \tag{1.4}
$$

where R_{ij} are rational functions whose coefficients depend on the elements of the tableau (1.2) (see e.g. [7]). For explicit methods, with $\alpha_{ij} = 0$, $i \leq j$, the R_{ij} are polynomials of degree $\leq s$. The true solution of course satisfies a similar recursion

$$
\begin{bmatrix} p(t_n + h) \\ q(t_n + h) \end{bmatrix} = \begin{bmatrix} \cos h\lambda & -\lambda \sin h\lambda \\ \lambda^{-1} \sin h\lambda & \cos h\lambda \end{bmatrix} \begin{bmatrix} p(t_n) \\ q(t_n) \end{bmatrix}. \tag{1.5}
$$

It is reasonable to demand that, for small h, the *amplification matrix* in (1.4) possesses eigenvalues of unit modulus; an eigenvalue of modulus > 1 would be associated with exponentially growing numerical solutions and an eigenvalue of modulus < 1 would be associated with exponentially decreasing numerical solutions. In what follows we say that an RKN method is *nondissipative,* if the

corresponding amplification matrix has eigenvalues of unit modulus when λ is real and h small. This terminology is taken from [7]; in the Russian literature the alternative term ω-stability appears to be in use [14]. In any case we feel that the notion of nondissipativity is familiar in numerical analysis and widely employed in connection with hyperbolic problems.

On the other hand, an RKN method is called *symplectic* [13], [6] if, whenever it is applied to a Hamiltonian problem of the form (1.1) (with $\mathbf{f}$ the gradient of a scalar function), the Jacobian matrix of the mapping $(\mathbf{p}^n, \mathbf{q}^n) \to (\mathbf{p}^{n+1}, \mathbf{q}^{n+1})$ satisfies the condition

$$\frac{\partial(\mathbf{p}^{n+1}, \mathbf{q}^{n+1})}{\partial(\mathbf{p}^n, \mathbf{q}^n)}^T J \frac{\partial(\mathbf{p}^{n+1}, \mathbf{q}^{n+1})}{\partial(\mathbf{p}^n, \mathbf{q}^n)} \equiv J, \tag{1.6}$$

where J is the $2d \times 2d$ matrix

$$J = \begin{bmatrix} 0 & I \\ -I & 0 \end{bmatrix}.$$

The condition (1.6) is a characteristic geometric property satisfied by the Jacobian matrix of the true solution $(\mathbf{p}(t_n), \mathbf{q}(t_n)) \to (\mathbf{p}(t_n + h), \mathbf{q}(t_n + h))$. The conditions on the tableau coefficients for an RKN method to be *symplectic* were first derived by Suris [15] and are by now well known, see, among others, [1], [2], [3], [11], [12]. Explicit symplectic RKN methods of order four appear to be competitive with standard software when integrating Hamiltonian problems [2]. However, the class of explicit, symplectic RKN methods is rather small and to achieve high order it is necessary to resort to formulae with many stages [1]. As a consequence, currently available high-order, explicit RKN methods are rather inefficient [3]. The question arises of whether the requirement of symplecticness could not be somewhat relaxed while retaining some of the favourable qualitative features of symplectic integrators, cf. [10]. In this paper we show (see the final Section 3) that the property of nondissipativity is, in this connection, too weak: nondissipative RKN methods do not share the advantages of symplectic RKN methods. This is of special interest because of two reasons. First, it is our experience that some users of numerical methods wrongly take as synonymous the terms nondissipativity and symplecticness. Secondly, it turns out that (see Section 2), for RKN methods, nondissipativity is necessary and sufficient for symplecticness in *linear problems.*

2 Constructing a nondissipative method.

The following result will be used.

THEOREM 1. *For a consistent Runge-Kutta-Nyström method (1.2)–(1.3) the following conditions are equivalent.*

(i) The method is nondissipative.

(ii) The method is symplectic when applied to linear Hamiltonian problems of the form (1.1).

(iii) The amplification matrix of the method has determinant unity, i.e.,

$$R_{11}(z)R_{22}(z) - R_{12}(z)R_{21}(z) \equiv 1. \tag{2.1}$$

Proof. The equivalence between (i) and (iii) is shown by Suris [14]. The problem (1.1) is linear and Hamiltonian if $\mathbf{f}(\mathbf{q})$ is of the form $S\mathbf{q}$, with S a constant $d \times d$ symmetric matrix. A step of the RKN method for such a system reads (cf. (1.4))

$$\begin{bmatrix} \mathbf{p}^{n+1} \\ \mathbf{q}^{n+1} \end{bmatrix} = \begin{bmatrix} R_{11}(-h^2S) & h^{-1}R_{12}(-h^2S) \\ hR_{21}(-h^2S) & R_{22}(-h^2S) \end{bmatrix} \begin{bmatrix} \mathbf{p}^{n} \\ \mathbf{q}^{n} \end{bmatrix},$$

and therefore the relevant Jacobian matrix is

$$\begin{bmatrix} R_{11}(-h^2S) & h^{-1}R_{12}(-h^2S) \\ hR_{21}(-h^2S) & R_{22}(-h^2S) \end{bmatrix}.$$

Substitution in (1.6) readily makes apparent the equivalence between (ii) and (iii). □

Note in particular that all symplectic (consistent) RKN methods are nondissipative.

We undertook the task of constructing a nondissipative, explicit RKN method of order four with three stages. There are nine parameters to be determined, namely b_i, γ_i, $i = 1, 2, 3$, α_{21}, α_{31}, α_{32}. These nine unknowns should satisfy the following requirements:

(i) The seven conditions that impose order four, [6], Section II.14, [13], Section 4.5.

(ii) The condition (2.1) that guarantees nondissipativity. For an explicit method with $s = 3$, the left-hand side of (2.1) is a polynomial $P(z)$ of degree six and therefore (2.1) demands that the coefficients of z^i in $P(z)$, $i = 1, \ldots, 6$ vanish, while the coefficient of z^0 should be 1. Thus, apparently, nondissipativity brings in seven scalar equations. However, it turns out that the conditions relative to z^i, $i = 0, 1, 2$ are implied by the order conditions for order ≥ 4. This comes about because for a method of order r the entries of the amplification matrix in (1.4) differ in $O(h^{r+1})$ terms from those of the matrix in (1.5). Since the latter has unit determinant, the amplification matrix has determinant $1+O(h^{r+1})$. As a result, the left-hand side of (2.1) is $1 + O(z^{[(r+1)/2]})$ for methods of order r. This leaves in (2.1) the four conditions corresponding to z^i, $i = 3, 4, 5, 6$. A little algebra shows that the conditions for $i = 4, 5, 6$ are implied by the structure of the method. The conclusion is that nondissipativity is ensured by the equation that imposes that the coefficient of z^3 in the left-hand side of (2.1) vanishes.

We have thus found a system with eight equations for nine unknowns. We are interested in solutions of this system that corresponds to methods with small error constants. We wrote the error constants $\dot{A}$ and A corresponding respectively to the p and q variables (see [13], Section 8.5.3 for the definition) as functions

of the nine unknown parameters. Then we used the NAG Library optimization subroutine E04UCF to minimize $\sqrt{\dot{A}^2 + A^2}$, subject to the eight equality constraints that impose order $r = 4$ and nondissipativity. Also the unknown parameters were bounded by inequality constraints $-5 \leq b_i, \alpha_{ij}, \gamma_j \leq 5$. The subroutine was run with 10,000 randomly chosen initial guesses. Of all methods found we kept the one with smallest objective function. Since the tableau coefficients obtained in this way do not exactly solve the equality constraints, we fixed the values of one of the coefficients and used the values of the remaining eight as initial guesses of a quadruple precision Newton iteration for the eight equations being solved. In this way, we arrived at the method

$$\begin{aligned}
b_1 &= 0.35873776474082084915 \\
b_2 &= 0.24851004590527121138 \\
b_3 &= 0.39275218935390793947 \\
\gamma_1 &= 0.16227389678337366829 \\
\gamma_2 &= 0.46956286655940066010 \\
\gamma_3 &= 0.82773602357979500167 \\
\alpha_{21} &= 0.14555733200712389602 \\
\alpha_{31} &= 0.21110902166846736304 \\
\alpha_{32} &= 0.12114681533245518567
\end{aligned}$$

with error constants $\dot{A} = 2.7 \times 10^{-3}$ and $A = 2.8 \times 10^{-3}$.

The nondissipative method has been compared with an explicit, symplectic RKN method with the same order and same number of stages. This symplectic method, first found by Forest and Ruth [5] and, independently, by Candy and Rozmus [4] has

$$\begin{aligned}
b_1 = \Omega, \quad & b_2 = 1 - 2\Omega, \quad & b_3 = \Omega, \\
\gamma_1 = \Omega/2, \quad & \gamma_2 = 1/2, \quad & \gamma_3 = 1 - \Omega/2, \\
\alpha_{21} = b_1(\gamma_2 - \gamma_1), \quad & \alpha_{31} = b_1(\gamma_3 - \gamma_1), \quad & \alpha_{32} = b_2(\gamma_3 - \gamma_2),
\end{aligned}$$

with

$$\Omega = (2 + 2^{1/3} + 2^{-1/3})/3.$$

An explicit, symplectic RKN method with three stages has six free parameters b_i, γ_i, $i = 1, 2, 3$ and to achieve order four there are six symplectic order conditions [1]. This leaves no free parameter after imposing the order conditions. In the nondissipative case, with $s = 3$, $r = 4$, there are, as we saw, nine unknown coefficients and eight equations, leaving one free parameter. It is therefore reasonable to expect that the nondissipative method we constructed has error constants significantly smaller than those of the reference symplectic integrator. In fact, the latter has ([13], Table 9.1) $\dot{A} = 1.2 \times 10^{-1}$, $A = 3.7 \times 10^{-2}$, which is far from satisfactory; the literature contains explicit, symplectic RKN methods with $r = 4$, $s > 3$ that are substantially more efficient than the symplectic method used here, see e.g. [13], Section 9.1 and [8], [9]. Thus in the comparisons presented in the final section we are being *biassed against symplectic integrators.*

3 Numerical experiments.

The methods described in the preceding section were tried in the test problems used in the comparisons of [13], Section 9.1. Only the results corresponding to the Kepler test problem will be reported; the main conclusion as to the relative merit of the algorithms does not depend on the specific test problem.

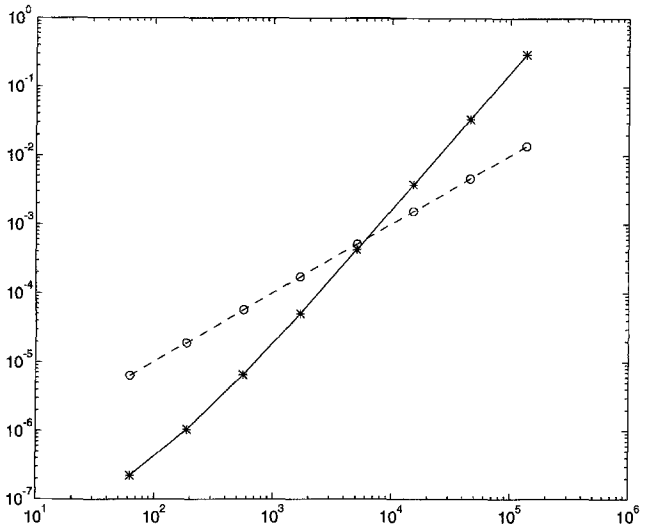

Figure 3.1: Euclidean norm of the error against t, when $h = 2\pi/1024$.

The Kepler problem used here has $d = 2$, $\mathbf{f}(\mathbf{q}) = -(1/|\mathbf{q}|^3)\mathbf{q}$ and initial condition

$$p_1 = 0, \quad p_2 = \sqrt{\frac{1+e}{1-e}}, \quad q_1 = 1-e, \quad q_2 = 0, \quad e = 0.5.$$

The solution is 2π-periodic and, as in [13], the integration covers from $t = 0$ to $t = 21870 \times 2\pi$.

Fig. 3.1 depicts in a log-log scale the Euclidean norm of the error against t, when $h = 2\pi/1024$. The solid line corresponds to the nondissipative method and the broken line to the symplectic method. By measuring the slopes of the lines, it is concluded that in the symplectic method the norm of the error is a *linear* function of t, a behaviour typical of symplectic integrators, see [2]. On the other hand the error growth in the nondissipative method is *quadratic* in t. When t is small, the nondissipative method is more accurate than the symplectic algorithm; this is explained by the relative size of the error constants. However errors build up more rapidly in the nondissipative method, which for $t > 10000$ is less accurate than the symplectic scheme.

Figs. 3.2 and 3.3 correspond to $h = 2\pi/2048$ and $h = 2\pi/4096$ respectively. We observe that the cross-over time where the nondissipative algorithm becomes

less accurate than the symplectic scheme is doubled each time h is halved. This is consistent with the analysis in [2]

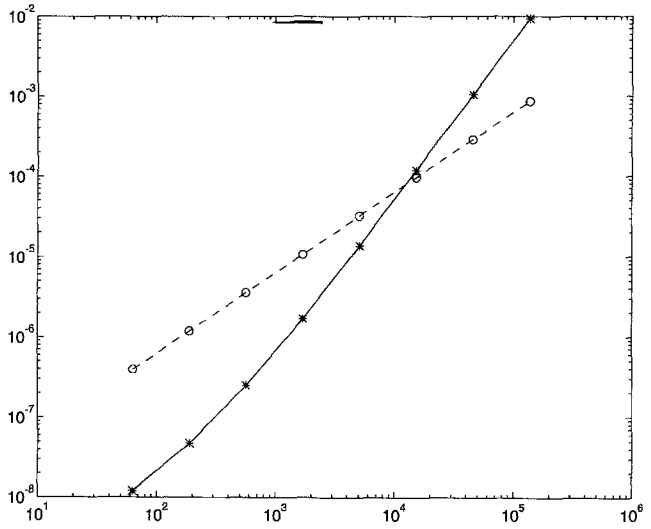

Figure 3.2: Euclidean norm of the error against t, when $h = 2\pi/2048$.

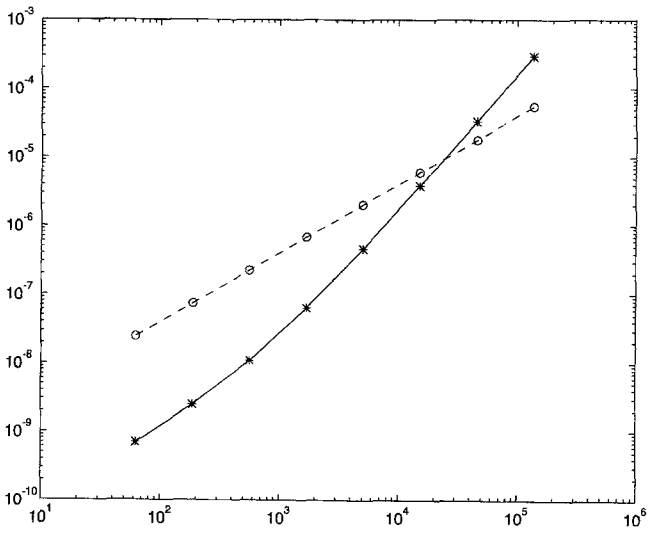

Figure 3.3: Euclidean norm of the error against t, when $h = 2\pi/4096$.

The conclusion is that, in long time integrations of Hamiltonian problems, nondissipative methods do not in general share the good error propagation mechanism typical of symplectic integrators. Even an inefficient symplectic formula is capable of outperforming the nondissipative method with small error constants we constructed.

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