

SYMMETRIC LINEAR MULTISTEP METHODS

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Dedicated to the memory of Germund Dahlquist

Abstract.

Some important early contributions of Germund Dahlquist are reviewed and their impact to recent developments in the numerical solution of ordinary differential equations is shown. This work is an elaboration of a talk presented in the Dahlquist session at the SciCADE05 conference in Nagoya.

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1 Introduction.

For the numerical solution of ordinary differential equations, symmetric integration methods (trapezoidal rule, midpoint rule, leapfrog method) appear very naturally as simple low order discretisations, and they are known since the beginning of numerical integration. High order symmetric multistep methods were found more or less by accident, when Dahlquist searched for the most accurate representative in the class of general linear multistep methods.

These symmetric methods did not receive much attention over many years. For nonstiff differential equations, Adams, Störmer, and Runge–Kutta methods have been in use with much success, and there was no reason for switching to symmetric integrators. For stiff differential equations, symmetric methods are penalised because of their bad damping at infinity.

About 20 years ago, the interest in qualitatively correct integrations grew rapidly. One became aware that symplectic integrators for Hamiltonian systems and symmetric methods for time-reversible problems often have a much better behaviour for integrations of long times.

It was a publication by Quinlan & Tremaine [11] in 1990 that revived the study of symmetric multistep methods. There, an excellent performance of such methods is reported for simulations of the outer solar system. Recently, much new insight into their longtime behaviour has been gained. The long-term stability of parasitic solution components, the near conservation of quadratic invariants, and the near symplecticity are now well understood for special important situations.

The aim of this article is to show how the ideas of Dahlquist's early work on symmetric linear multistep methods appear again in the present research and how they are further developed to provide new insight.

2 Role of growth parameters (Dahlquist's talk in Freiburg 1951)

At a conference in Freiburg im Breisgau, Dahlquist presented one of his first discoveries concerning the numerical integration of ordinary differential equations. It is published in the one-page paper [1], and gives a clear indication of how linear multistep methods have to be analysed. We quote from [4], where the essentials of his talk are reproduced:

This particular analysis is concerned with the application of the leapfrog method,

$$(2.1) \quad y_{n+1} = y_{n-1} + 2hf(y_n, t_n)$$

for the system, $dy/dt = f(y, t)$, $y(0) = c$. The local truncation error per unit of time is, $p(t) \approx h^2 y^{(3)}/6$. I show, by a somewhat heuristic (though not very sloppy) argument, loc. cit., that the error may be decomposed according to the formula,

$$(2.2) \quad y(t_n) - y_n \approx u(t_n) + av(t_n) + b(-1)^n w(t_n),$$

where u, v, w are solutions of the differential equations

$$(2.3) \quad \begin{aligned} du/dt &= J(t)u + p(t), & u(0) &= 0, \\ dv/dt &= J(t)v, \\ dw/dt &= -J(t)w, \end{aligned}$$

where $J(t) = \partial f / \partial y$ is the Jacobian evaluated at $(t, y(t))$, ... For other (two-step) methods studied nothing is changed in (2.3) except for the expression for the local truncation error, but the last equation of (2.3) reads,

$$(2.4) \quad dw/dt = cJ(t)w,$$

where c is a constant characteristic for the method (later called a growth parameter).

If the growth parameter c is negative (and this is typically the case for symmetric linear multistep methods, cf. [9]), the differential equations for $v(t)$ and $w(t)$ in (2.3) have often an opposite stability behaviour. E.g., for $dy/dt = \lambda y$ with $\Re \lambda < 0$, the solution is contractive but the oscillating term in the error formula grows exponentially with time which makes the method useless on longer time intervals.

But what happens with Hamiltonian systems which can be stable for positive and negative time? For the problem $dy/dt = \lambda y$, $\Re \lambda = 0$ (harmonic oscillator) the differential equation (2.4) is stable whatever the sign of the growth parameter c is, and the leapfrog method (2.1) can be safely used as numerical integrator. The following example illustrates that this behaviour does not generalise to nonlinear Hamiltonian systems.

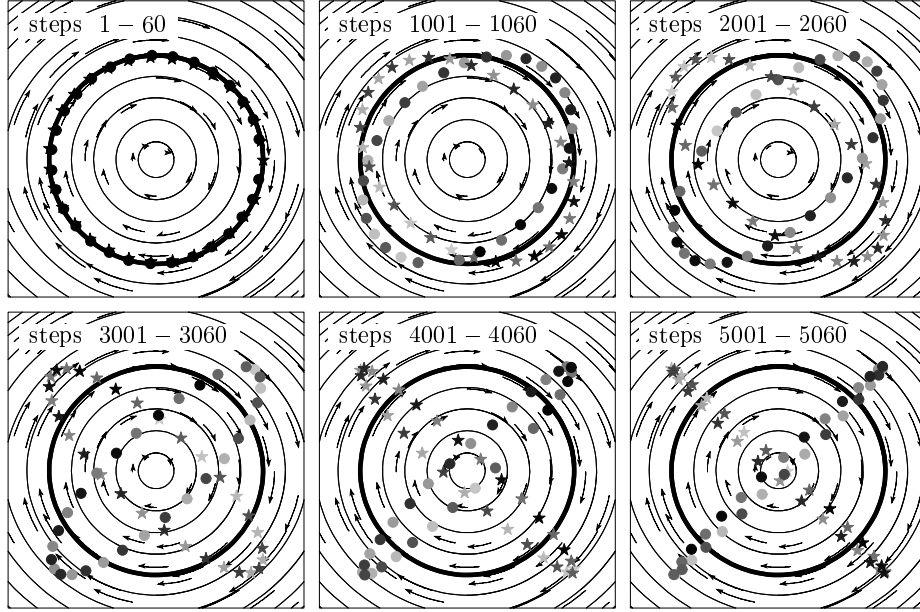


Figure 2.1: Leapfrog method applied to the pendulum equation, step size $h = \pi/15$, initial value $(q_0, p_0) = (0.779, 0)$, starting approximation (q_1, p_1) computed with the explicit Euler method.

EXAMPLE 2.1. Consider the equations for the mathematical pendulum

$$\dot{q} = p, \quad \dot{p} = -\sin q$$

with initial values $(q_0, p_0) = (0.779, 0)$. The exact solution (drawn as thick line in the pictures of Figure 2.1, q horizontal, p vertical) is very close to a circle as for the harmonic oscillator. The numerical solution of the leapfrog method with step size $h = \pi/15$, which corresponds to 30 approximations per period, is shown in Figure 2.1. The approximations (q_n, p_n) with even n are plotted as circles, those with odd n as stars. Increasing n is indicated by increasing darkness.

Only during a few periods, the numerical solution remains close to the exact solution (first picture in Figure 2.1). It drifts away when longer time integrations are considered (pictures two to six). We also observe that the approximations with even n (circles) lie on a smooth curve, and those with odd n (stars) lie on a different smooth curve. This agrees very well with formula (2.2) and indicates that the parasitic term $w(t)$ grows linearly with time.

This disappointing behaviour of the leapfrog method on one of the most simple Hamiltonian systems may discourage people from considering linear multistep methods for long-time integrations. We shall see later in this article that there exists a class of multistep methods (for second order differential equations) for which the parasitic components remain bounded and small over long times. Methods in this class are therefore well suited for long-time computations of Hamiltonian systems.

3 General linear multistep methods (Dahlquist 1956)

The impressive publication [2] by Dahlquist begins with the sentence:

Statement of the problem. Consider a class of difference equations

$$(3.1) \quad \alpha_k y_{n+k} + \alpha_{k-1} y_{n+k-1} + \dots + \alpha_0 y_n = h(\beta_k f_{n+k} + \dots + \beta_0 f_n).$$

This was the birth of the general formulation of linear multistep methods for first order differential equations. A few years later, Henrici [9] writes in his classical textbook “... *this approach, which was first adopted by Dahlquist [1956], leads to a mathematically well-rounded theory. It also leads to the discovery of new integration formulas which could not be obtained by the heuristic methods ...*”

It is interesting to read further in the introduction of the article [2]:

... one may ask whether it would not be possible to make use of the information from the preceding points in a much more efficient manner by choosing a more complicated formula ... This question was the starting point of the writer's investigations. The main result is rather negative (Theorem 4), but there are new formulas of this general class which are at least comparable to the classical numerical methods ...

Today, everybody would be proud having written such an influential article. Dahlquist was apparently disappointed with his findings. By introducing the coefficients α_i and β_i (the more complicated formula) he expected to be able to construct more accurate formulas having an order much higher than the classical methods like those of Adams. He proved an order bound for stable methods, and he found that the methods of maximum order $k + 2$ are necessarily symmetric. His analysis of the global error (see Sect. 1) indicates the presence of parasitic solution components with symmetric multistep methods, so that he did not further promote these methods. In a letter to the author (22. Feb. 1998) Dahlquist writes: “*In 1984 a graduate student, who took my ODE class at Stanford, wanted to work with symmetric multistep methods. I discouraged him, ...*”.

The article [2] contains many interesting investigations: the study of strong and weak instability, of stable convergence, the role of the generating polynomials

$$\rho(\zeta) = \alpha_k \zeta^k + \alpha_{k-1} \zeta^{k-1} + \dots + \alpha_0, \quad \sigma(\zeta) = \beta_k \zeta^k + \beta_{k-1} \zeta^{k-1} + \dots + \beta_0,$$

the construction of high order multistep methods, the famous Dahlquist order barrier of stable multistep methods, and the symmetry for methods of maximal order. It is worth mentioning that not only the methods and the analysis of Dahlquist are still relevant, but even the notation α_j , β_j for the coefficients and $\rho(\zeta)$, $\sigma(\zeta)$ for the generating polynomials are used until now in nearly all publications concerning multistep methods.

4 Dahlquist's thesis (1958) and second order differential equations

The work initiated in the publication [2] is further developed in Dahlquist's thesis, which was published in 1958 by Almqvist & Wiksell, Uppsala, and then also distributed as Nr. 130 of the Transactions of the Royal Institute of Technology, Stockholm, Sweden, in 1959 [3].

The thesis of Dahlquist presents a complete theory (accuracy, stability, convergence) for general linear multistep methods, it introduces the logarithmic norm of matrices and studies differential inequalities in view of a convergence analysis, and it considers various extensions of the results of [2].

The extension which interests us most is that to second order differential equations $\ddot{y} = f(y)$. Dahlquist proposes to consider the general formula

$$(4.1) \quad \alpha_k y_{n+k} + \dots + \alpha_0 y_n = h^2 (\beta_k f_{n+k} + \dots + \beta_0 f_n).$$

The stability of such a formula requires that the zeros of the generating polynomial $\rho(\zeta) = \alpha_k \zeta^k + \dots + \alpha_0$ are all in the unit disc and those on its border have a multiplicity less or equal to *two*. It is proved in [3] that the order p of a stable method (4.1) satisfies $p \leq k + 2$, and one has $p = k + 2$ only if k is even and the method is symmetric, i.e.,

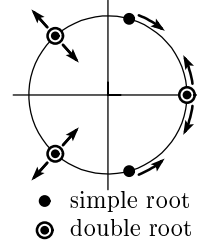
$$\alpha_{k-i} = \alpha_i, \quad \beta_{k-i} = \beta_i$$

Let us discuss in more detail the weak instability (or weak stability) of symmetric formulas. This is essential for the rest of this article. We thus consider the differential equation of the harmonic oscillator $\ddot{y} + \omega^2 y = 0$ for which (4.1) becomes a linear difference equation with characteristic polynomial

$$(4.2) \quad \rho(\zeta) + (h\omega)^2 \sigma(\zeta).$$

Denoting the zeros of this polynomial by $\zeta_j(h\omega)$, the numerical solution is given by $y_n = c_1(h\omega)\zeta_1(h\omega)^n + \dots + c_k(h\omega)\zeta_k(h\omega)^n$. Since the coefficients of (4.2) are real, roots appear in pairs, and the symmetry implies that with $\zeta_j(h\omega)$ also $1/\zeta_j(h\omega)$ is a root. Consequently,

- if $\zeta_j(0) \neq 1$ is a simple root of $\rho(\zeta)$, the root $\zeta_j(h\omega)$ of (4.2) remains on the unit circle as long as it does not interfere with another root; in this situation there is *no weak instability*.
- if $\zeta_j(0) \neq 1$ is a double root, $\zeta_j(h\omega)$ can leave the unit disc and an exponential error growth is possible in this case.



By consistency of the formula, the principal roots $\zeta_{1,2}(h\omega)$ approximate $e^{\pm ih\omega}$ and remain on the unit circle for sufficiently small $h\omega$. Dahlquist mentions that for even k there always exists a method of maximum order $k + 2$ which shows no weak instability. In fact, the polynomial $\rho(\zeta)$ can be chosen arbitrarily satisfying the above stability requirements, and then $\sigma(\zeta)$ is uniquely determined by the order conditions.

After Dahlquist's work, symmetric multistep methods did not receive much attention for a long time. Nearly 20 years later, Lambert & Watson [10] studied multistep methods for which the numerical solution remains close to a periodic orbit of the linear test equation. A revival of symmetric multistep methods (4.1) suddenly came through the work of Quinlan & Tremaine [11] who report an excellent performance of such methods for long-time integrations in celestial mechanics.

5 Multistep methods for long-term calculations

For a justification of correct long-time integrations in Hamiltonian systems, symmetric linear multistep methods have two major obstacles:

- the smooth part in the numerical solution (which corresponds to $u(t)+av(t)$ in the error formula (2.2)) has to satisfy a good long-time behaviour as it is known from symplectic one-step methods;
- the parasitic solution components (the oscillating term in (2.2)) has to remain bounded and small over long times.

In the spirit of Dahlquist's error analysis of Sect.1 we aim in writing the numerical solution of a stable symmetric multistep method (4.1) as

$$(5.1) \quad y_n = v(nh) + \sum \zeta_j^n w_j(nh).$$

Here, the sum is over the zeros $\zeta_j \neq 1$ of $\rho(\zeta)$ and over products of them (the sum is finite if all ζ_j are roots of unity). The function $v(t)$ approximates the exact solution of the differential equation, and the $w_j(t)$ are so-called parasitic solution components.

Backward error analysis. For the study of the long-time behaviour of numerical solutions, one needs a good knowledge of the functions $v(t)$ and $w_j(t)$. This is achieved by a backward error analysis (see [6] for methods (3.1), [7] and [8] for methods (4.1)). Inserting (5.1) into the multistep formula, expanding in powers of h around $t = t_n = nh$, and comparing the coefficients of ζ_j^n , one finds that the function $v(t)$ is the formal solution of a differential equation which is a perturbation of $\ddot{y} = f(y)$, and the $w_j(t)$ are formal solutions of

$$(5.2) \quad \begin{aligned} \ddot{w}_j &= \mu_j f'(v) w_j + \dots & \text{if } \rho(\zeta_j) = \rho'(\zeta_j) = 0, \rho''(\zeta_j) \neq 0, \\ \dot{w}_j &= \mu_j h f'(v) w_j + \dots & \text{if } \rho(\zeta_j) = 0, \rho'(\zeta_j) \neq 0, \\ w_j &= \mu_j h^2 f''(v)(w_k, w_l) + \dots & \text{if } \zeta_j = \zeta_k \zeta_l, \rho(\zeta_j) \neq 0, \end{aligned}$$

where $\mu_j = \sigma(\zeta_j) \kappa! / (\zeta_j^\kappa \rho^{(\kappa)}(\zeta_j))$ with $\kappa = 2$ in the first equation, $\kappa = 1$ in the second, and $\kappa = 0$ in the third equation. These constants are related to the growth parameter of equation (2.4). Since the differential equation $\ddot{z} = \mu f'(y)z$ with $\mu \neq 1$ can have a completely different long-time behaviour than that of $\ddot{y} = f(y)$, double roots of $\rho(\zeta)$ should be avoided. This is in agreement with the linear stability analysis of Sect. 4. The presence of the factors h and h^2 in the modified equations for the remaining cases encourages us to study further the long-time behaviour of linear multistep methods.

Hamiltonian systems. For the rest of this article we consider linear multistep methods (4.1) applied to a Hamiltonian system

$$(5.3) \quad \ddot{y} = -\nabla U(y)$$

written as a second order differential equation. Although general potentials $U(y)$ can be considered, we have in mind N -body problems and high accuracy computations in celestial mechanics.

The study of the long-time behaviour requires a good knowledge of the modified equations (5.2), and it is not sufficient to consider the dominant term. This has been elaborated in [7], see also Chap. VX of [8]. It can be shown that under suitable assumptions the modified equations inherit the Hamiltonian structure of the differential equation (5.3). This permits one to obtain the following result which is taken from [7].

THEOREM 5.1. *Consider a linear multistep method (4.1) applied to the Hamiltonian system (5.3), and assume that*

- *the potential function $U(y)$ is defined and analytic in an open neighbourhood of a compact set K ;*
- *the method (4.1) is symmetric, stable, of order p , and such that the zeros of the ρ -polynomial are all simple and on the unit circle (with the exception of $\zeta_1 = 1$ which is a double zero);*
- *the starting approximations y_0, y_1, \dots, y_{k-1} are $\mathcal{O}(h^{p+1})$ close to the exact solution of the problem (h is the step size).*

As long as the numerical solution stays in the compact set K and on intervals of length $T = \mathcal{O}(h^{-p-2})$ (if no root of $\rho(\zeta)$ other than 1 can be written as the product of two other roots, on intervals of length $T = \mathcal{O}(h^{-2p-3})$) we have

- *the parasitic solution components $w_j(t)$ in the representation (5.1) are bounded and of size $\mathcal{O}(h^{p+1})$ on intervals of length T ;*
- *the total energy $H(y, \dot{y}) = \frac{1}{2}\dot{y}^T \dot{y} + U(y)$ is conserved up to $\mathcal{O}(h^p)$ (without drift) on intervals of length T ; the derivative approximation \dot{y}_n is computed a posteriori with a difference formula of order p ;*
- *quadratic first integrals of the form $L(y, \dot{y}) = \dot{y}^T A y$ (for example the angular momentum in N -body problems) are conserved up to $\mathcal{O}(h^p)$ (without drift) on intervals of length T ;*
- *if (5.3) is completely integrable and if the initial values satisfy a certain non-resonance condition, then we have for $t_n = nh$*

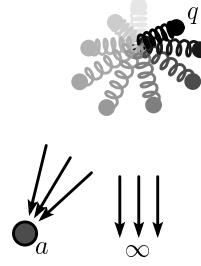
$$\begin{aligned} (y_n, \dot{y}_n) - (y(t_n), \dot{y}(t_n)) &= \mathcal{O}(th^p) \\ I(y_n, \dot{y}_n) - I(y_0, \dot{y}_0) &= \mathcal{O}(h^p) \end{aligned}$$

on intervals of length T ; here, $I(y, \dot{y})$ denotes a first integral of the system that depends only on the action variables.

With exception of the property of exact conservation of quadratic first integrals, linear multistep methods (4.1) without weak instability share the same good long-time behaviour with symplectic one-step methods.

EXAMPLE 5.1 (SPRING PENDULUM WITH GRAVITY AND ATTRACTION). To illustrate that methods studied in Theorem 5.1 usually have a better long-term behaviour than symmetric non-symplectic one-step methods, we consider the mechanical system (5.3) with two degrees of freedom (i.e., $y = (y_1, y_2) \in \mathbb{R}^2$) and with the potential function (cf. [5])

$$U(y) = \frac{\omega^2}{2} (\|y\| - 1)^2 + y_2 - \frac{1}{\|y - a\|},$$



where $\omega = 2$ and $a = (-3, -5)^T$. Initial values are $y_1(0) = 0$, $y_2(0) = 1$, $\dot{y}_1(0) = -1$, and $\dot{y}_2(0) = -0.5$, which correspond to the upright position of the spring (light grey in the picture). The velocity is sufficiently large so that the pendulum turns around the fixed origin (increasing darkness).

As numerical integrator for this problem we consider the explicit linear multistep method of order 4,

$$y_{n+4} - y_{n+3} - y_{n+1} + y_n = \frac{h^2}{4} (5f_{n+3} + 2f_{n+2} + 5f_n),$$

and we use sufficiently accurate starting approximations for y_1 , y_2 , and y_3 . The upper picture of Figure 5.1 shows the error in the energy for a computation with step size $h = 0.03$. In agreement with our theorem, no drift in the energy is visible, and the error remains $\mathcal{O}(h^4)$ small on extremely long time intervals.

For comparison, we also apply the 3-stage Lobatto IIIB method, which is a symmetric but non-symplectic implicit Runge-Kutta method (see [8] for the coefficients). We apply this method to the same problem with step size $h = 0.09$

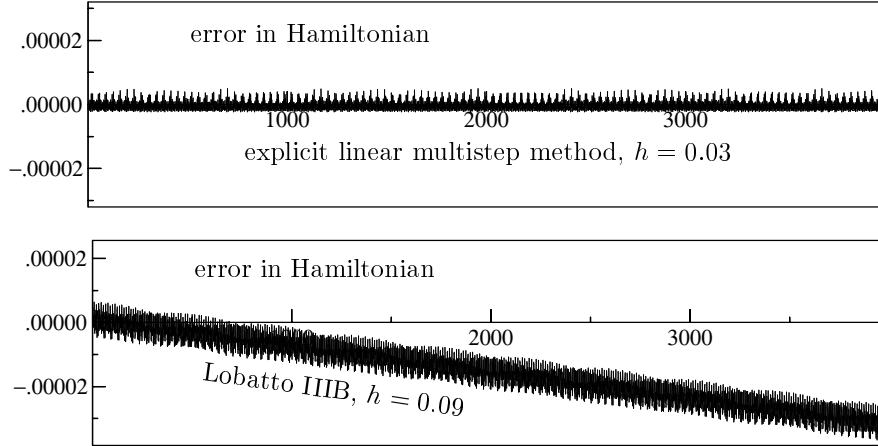


Figure 5.1: Energy error of numerical methods applied to the spring pendulum of Example 5.1

(notice that one step requires 3 function evaluations per iteration in solving the nonlinear Runge–Kutta equations). This time, there is a clear linear drift in the error of the total energy (lower picture of Figure 5.1). It should be mentioned that this linear drift disappears if one considers either attraction or gravity (but not both). In this situation, some symmetry is introduced in the problem.

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