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DAHLQUIST'S CLASSICAL PAPERS ON STABILITY THEORY *

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Abstract.

This text, which is based on the author's talk in honour of G. Dahlquist at the SciCade05 meeting in Nagoya, describes the two classical papers from 1956 and 1963 of Dahlquist and their enormous impact on the research of decades to come ; it also allows the author to present a personal testimony of his never ending admiration for the scientific and personal qualities of this great man.

AMS subject classification (2000): 65F05, 65F07.

Key words: Stability of multistep methods, A-stability.

1 Introduction.

"You know, I am a multistep man ... and don't tell anybody, but the first program I wrote for the first Swedish computer was a Runge-Kutta code ..."
(G. Dahlquist 1982, after 10 glasses of wine)

"Mr. Dahlquist, when is the spring coming ?"
"Tomorrow, at two o'clock."
(Weather forecast, Stockholm 1955)

The strong Fenno-Swedish tradition in complex and functional analysis gave Dahlquist during his studies the great intellectual strength, which then allowed him, after obtaining a job at the Swedish Board for Computing Machinery and working with the first Swedish computer (see citations), to become one of the revolutioneers of modern Numerical Analysis.

2 The First Dahlquist Barrier (1956, 1959).

"This work must certainly be considered as one of the great classics in numerical analysis"
(Å. Björk, C.-E. Fröberg 1985).

"And slowly came up these rho and sigma polynomials . . . " G. Dahlquist, private communication 1979).

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This first of Dahlquist's great papers [4] has been published before the birth of BIT. We therefore find it appropriate to reproduce in facsimile some parts in more detail. The paper starts right away with the definition of the general formula

CONVERGENCE AND STABILITY IN THE NUMERICAL INTEGRATION OF ORDINARY DIFFERENTIAL EQUATIONS

GERMUND DAHLQUIST

1. Introduction and summary

1.1. Statement of the problem. Consider a class of difference equations

$$\alpha_k y_{n+k} + \alpha_{k-1} y_{n+k-1} + \ldots + \alpha_0 y_n = h(\beta_k f_{n+k} + \ldots + \beta_0 f_n), \tag{1.1}$$

and gives a careful numerical analysis of the highest-order explicit two-step method, which, of course, every one who has seen the method definition and the order conditions, derives first:

1.2. A numerical example. Apply the formula

$$y_{n+2} = -4y_{n+1} + 5y_n + h(4f_{n+1} + 2f_n)$$

Apparently, the numerical solution is of no use and, curiously, the solution becomes better with the use of a *wrong* initial value (cases II):

n	CASE I (numerical solution)		CASE IIa (numerical solution)		CASE IIb ζ_1^n with six correct dec.	
	y_n	$10^6 \cdot$ error	y_n	$10^6 \cdot$ error		$10^6 \cdot$ error
0	1,000000	0	1,000000	0	1	
1	1,105171	0	1,105168	3	1,10516781	3
2	1,221384	19	1,221395	8	1,221396	7
3	1,349907	−48	1,349852	7	1,349847	12
4	1,491532	293	1,491787	38	1,491808	17
5	1,650001	−1280	1,648797	−76	1,648698	23
6	1,815963	6156	1,821623	496	1,822088	31
7	2,042538	−28785	2,015902	−2149	2,013713	40
8	2,089871	135670	2,215192	10349	2,225491	50
9	3,097662	−638059	2,507999	−48396	2,459541	62
10	−0,284254	3,002536	2,490202	228080	2,718205	77

Stability Analysis.

> "The main result is rather negative (Thm. 4), but there are new formulas of this general class which are at least comparable." (G. Dahlquist 1956.)

The disappointing behaviour of the above formula is then explained by the "parasitic" root -5 of the ρ-polynomial

$$\begin{aligned} \varrho(\zeta) &\equiv \alpha_k\zeta^k + \alpha_{k-1}\zeta^{k-1} + \ldots + \alpha_0\,, \\ \sigma(\zeta) &\equiv \beta_k\zeta^k + \beta_{k-1}\zeta^{k-1} + \ldots + \beta_0\,. \end{aligned}$$

Only *stable* methods, i.e., methods whose roots of ρ are inside the unit circle, with simple roots allowed on the boundary, are of interest. But then comes the great deception in Theorems 4a and 4b:

THEOREM 4a. *The degree p of a stable operator of order k can never exceed $k+2$. If an operator is stable, then the condition that $R(z)$ is an odd function is necessary and sufficient for the degree to be equal to $k+2$. All roots of $R(z)$ are then located on the imaginary axis. If k is odd, the degree of a stable operator cannot exceed $k+1$.*

THEOREM 4b. *If an operator of even order k is stable, then the conditions*

$$\alpha_\nu = -\alpha_{k-\nu}, \qquad \beta_\nu = \beta_{k-\nu} \tag{2.22}$$

are necessary and sufficient in order that it should be of maximum degree $k+2$. All roots of $\varrho(\zeta)$ then have unit modulus.

Dahlquist's Proof.

> "Although there exist many different proofs for the theorem the original published proof still appears very elegant,..." (R. Jeltsch, O. Nevanlinna 1985)

Since polynomials with roots in the negative half plane are easier to handle (they necessarily have all coefficients of the same sign) than polynomials with roots in the unit circle, we define new polynomials $R(z)$ and $S(z)$ with the greek-roman transformation

$$\zeta = (z+1)/(z-1), \qquad z = (\zeta+1)/(\zeta-1)\,,$$

$$R(z) = \left(\tfrac{1}{2}(z-1)\right)^k \varrho(\zeta) \equiv \sum_{j=0}^{k} a_j z^j\,,$$

$$S(z) = \left(\tfrac{1}{2}(z-1)\right)^k \sigma(\zeta) \equiv \sum_{j=0}^{k} b_j z^j\,.$$

for which the conditions of order p become

In these notations the relation (2.15) transforms into

$$R(z) - S(z)\log\frac{z+1}{z-1} \sim -C\left(\frac{2}{z}\right)^{p-k+1} \qquad (z\to\infty)\,, \tag{2.17}$$

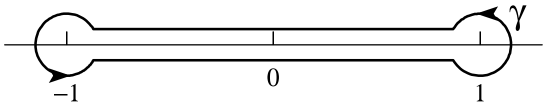
$$R(z)\left(\log\frac{z+1}{z-1}\right)^{-1} - S(z) \sim -C\left(\frac{2}{z}\right)^{p-k} \qquad (z\to\infty)\,. \tag{2.18}$$

However, the Laurent series of

$$\left(\log\frac{z+1}{z-1}\right)^{-1} = \frac{z}{2} - \sum_{\nu=0}^{\infty} \mu_{2\nu+1}\, z^{-(2\nu+1)}$$

has all coefficients $\mu_{2\nu+1} > 0$, which Dahlquist proves with a beautiful application of Cauchy's formula

$$\begin{aligned}\mu_{2\nu+1} &= -\frac{1}{2\pi i}\int_C z^{2\nu}\left(\log\frac{z+1}{z-1}\right)^{-1} dz\\ &= -\frac{1}{2\pi i}\int_{-1}^{1} x^{2\nu}\left(\pi^2+\log^2\frac{1+x}{1-x}\right)^{-1}\cdot\\ &\quad\cdot\left(\left(-\pi i+\log\frac{1+x}{1-x}\right)-\left(\pi i+\log\frac{1+x}{1-x}\right)\right)dx\\ &= \int_{-1}^{1} x^{2\nu}\left(\pi^2+\log^2\frac{1+x}{1-x}\right)^{-1} dx > 0\,.\end{aligned}$$



Hence, because the coefficients of $R(z)$ all have the same sign, too, the only liberty for eliminating the highest terms in the Laurent expansion of (2.18) is essentially the choice of the polynomial $S(z)$. We have the *positive* result, that for each polynomial $R(z)$ we can have order k by suitably adjusting $S(z)$ in (2.18), and unfortunately also the *negative* result, that not much more is possible. Happily, the referee at that time did not refuse the paper, by saying that Adams' methods had existed for one hundred years and that apparently no significant practical progress seemed possible.

The theory was perfect from the beginning (see citation), became famous mainly through the book by Henrici [12], and even the latest textbooks, for example [10], cannot do much more than reproduce it with the same theorems and the same notations — just, perhaps, adding a picture (see above). Various generalizations have been published since then, in particular Reimer's order barrier for multi derivative multistep methods [18].

The next great paper of Dahlquist [5] extended the theory into various directions, in particular to second order equations; its contents and their consequences are described in [9] in this issue.

Finally, the theory contained the germs for what some years later became the second great adventure, to which we will turn now.

3 The Second Dahlquist Barrier (1963)

Around 1960, things became completely different and everyone became aware that the world was full of stiff problems. (G. Dahlquist in Aiken 1985)

"certainly one of the most influential papers ever published in BIT" (Å. Björk, C.-E. Fröberg 1985).

A SPECIAL STABILITY PROBLEM FOR LINEAR MULTISTEP METHODS*

GERMUND G. DAHLQUIST

Abstract.

The trapezoidal formula has the smallest truncation error among all linear multistep methods with a certain stability property. For this method error bounds are derived which are valid under rather general conditions. In order to make sure that the error remains bounded as $t \to \infty$, even though the product of the Lipschitz constant and the step-size is quite large, one needs not to assume much more than that the integral curve is uniformly asymptotically stable in the sense of Liapunov.

I didn't like all these "strong", "perfect", "absolute", "generalized", "super", "hyper", "complete" and so on in mathematical definitions, I wanted something neutral; and having been impressed by David Young's "property A", I chose the term "A-stable".
(G. Dahlquist, private communication, 1979).

Stiff equations with large Lipschitz constants require the famous definition of A-stable methods:

DEFINITION. *A k-step method is called A-stable, if all solutions of* (1.2) *tend to zero, as $n \to \infty$, when the method is applied with fixed positive h to any differential equation of the form,*

$$dx/dt = qx\,, \qquad (1.8)$$

where q is a complex constant with negative real part.

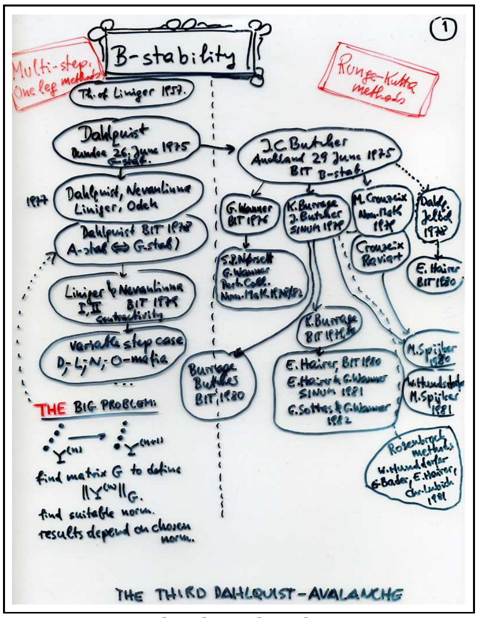
and the stability analysis now involves *both* polynomials ρ and σ and we have an even more disappointing result:

Theorem 2.2. *The order, p, of an A-stable linear multistep method cannot exceed 2. The smallest error constant, $c^* = \frac{1}{12}$, is obtained for the trapezoidal rule, $k=1$, with the generating polynomials (2.2).*

This famous theorem[1] became known as the "second Dahlquist barrier" and Sweden became *the* expert country for stiff problems:

> "Talking on stiff differential equations in Sweden, is like carrying coals to Newcastle..."
>
> (W.L. Miranker, Göteborg 1975).

Second avalanche.



Third avalanche.

Figure 3.1: The second and the third Dahlquist avalanche (slides of the author, presented around 1980)

In order to give an impression of the enormous impact of this theory, we reproduce in Fig. 3.1 (left) a slide from a talk of the author given around 1980. A third "avalanche" then concerned the so-called G-stability of Dahlquist (1975) (Fig. 3.1, right), which is explained in more detail in Butcher's paper [3] in this issue.

[1] A student, who is blamed by his teacher for a lack of logical rigor in one of his writings, can argue, that even Dahlquist, in his most famous theorem, has forgotten to mention $p = 2$ in the sentence concerning "the smallest error constant".

Proofs of Dahlquist's Theorem.

> "I searched for a long time, finally Professor Lax showed me the Riesz-Herglotz theorem and I knew that I had my theorem.."
>
> (G. Dahlquist, private comm. 1979)

> **analytic functions. Following a suggestion of Professor P. D. Lax (oral communication), we shall use a variant of Riesz–Herglotz' theorem, cf.**

Here, fortunately, Dahlquist left something over to do for later generations. The nicest results were not found by people who stared at the ρ and σ polynomials, but who were looking for something completely different, i.e., tried to solve the

3 Conjectures : Ehle's conjecture [7] (1968) concerned the A-stability of Padé approximations to the exponential function, the stability functions of most implicit Runge-Kutta methods. After having proved that the diagonal and the first two subdiagonal entries were A-stable, he conjectured that all other approximations were *not* A-stable :

> are L-acceptable. Furthermore, evidence is given to suggest that these are the only L-acceptable Padé approximations to the exponential.

Nørsett's conjecture [17] (1975) concerned the points where their stability domain crosses the imaginary axis :

> **Conjecture.** Let $A_n^m(q)$ be the *different* approximations of the Padé table of order $m+n$. Let ut consider the $\widetilde{B}$-polynomial for these functions as a polynomial in $z=r^2$ of degree n in z. Then this polynomial has exactly ℓ nonzero positive zeros z_i, $i=1(1)\ell$ and $n-\ell$ zeros z_i with $z_i=0$, $i=\ell+1(1)n$ when
> $$m=n-\begin{cases}2\ell+1\\2\ell+2\end{cases},\qquad \ell\geqq 1.$$

The Daniel-Moore conjecture [6] (1970) concerned the A-stability of multistep methods using higher derivatives and reduced to the second Dahlquist barrier for $J=0$:

> order $(L+1)(2J+2)$. It is conjectured here that no A-stable method of the form of Eq. 5–6 can be of order greater than $2J+2$ and that, of those A-stable methods of order $2J+2$, the smallest error constant is exhibited by the *Hermite method* of Eq. 5–7.

The Daniel-Moore conjecture was 'disproved' by Genin (1974) [8] by giving A-stable methods of 'order' $2l+\min(l,k)-1$ and everybody thought that the conjecture was wrong. The following discovery of Jeltsch (1976) [14] was then a big surprise:

NOTE ON A-STABILITY OF MULTISTEP MULTIDERIVATIVE METHODS

ROLF JELTSCH

Abstract.

Daniel and Moore [4] conjectured that an A-stable multistep method using higher derivatives cannot have an error order exceeding $2l$. We confirm partly this con-

equivalent with the one commonly used. In all these methods proposed by Genin in the proof of Theorem 10 the stability polynomial $\varrho_0(\zeta)$, given by (1.2), has $\zeta = 1$ as a root with multiplicity $m = \min\{l,k\}$. It is easy to

Nørsett's conjecture was then the first to be cleared up — negatively: the Padé fraction $R_{0,6}$ was a counter-example. However, this paper showed the way to go: make a careful study of the roots of the, now so-called, E-polynomial and their relations with the position of the poles of $R(z)$, which were clearly interrelated.

4 Order Stars.

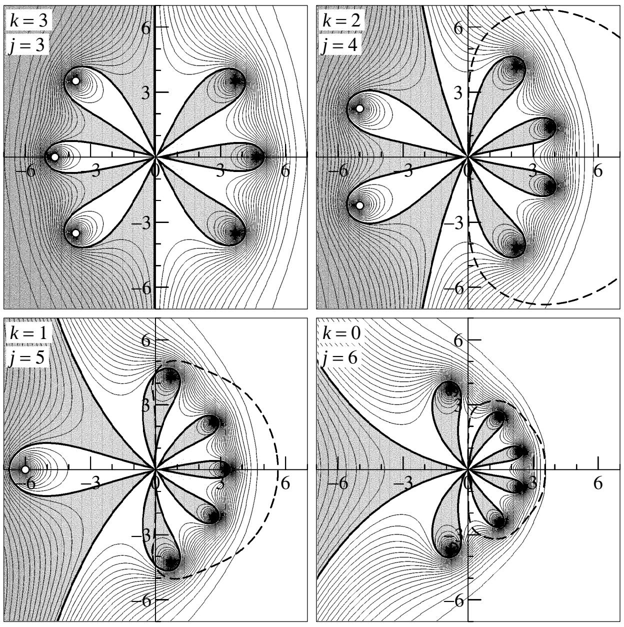


Figure 4.1: Order stars for some Padé fractions of the exponential funcion)

Trying to understand this relation led to the idea to look at the level curves of $|R(z)|$ — not compared to the constant 1 — but compared to the exponential function $|e^z|$. In this way the order stars were born [19], [20]. Apparently, G. Dahlquist liked them much:

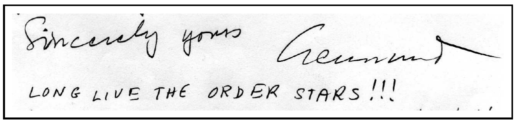


Fig. 4.1 indicates how these stars prove Ehle's Theorem, which itself extended a result of Birkhoff and Varga [2] (1965), of the A-stability for $k \le j \le k+2$ (first row), as well as the inverse result, which was Ehle's conjecture (second row).

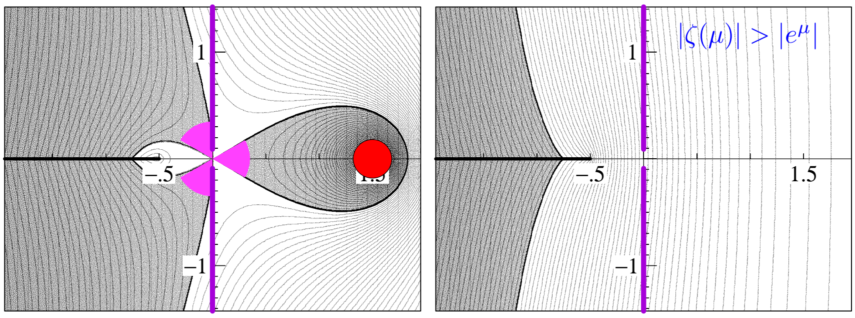
Multistep methods. Take as an example the BDF2 method

$$\frac{3}{2}y_{n+1} - 2y_n + \frac{1}{2}y_{n-1} = hf_{n+1}$$

for which the stability analysis leads to

$$y' = \lambda y, \quad \mu = h\lambda \quad \Rightarrow \quad \Big(\frac{3}{2} - \mu\Big)\zeta^2 - 2\zeta + \frac{1}{2} = 0.$$

We obtain an algebraic equation for ζ which leads to two roots $\zeta_{1,2}(\mu) = \frac{2\pm\sqrt{1+2\mu}}{3-2\mu}$ and have the order star on the corresponding Riemann surface



We have that

- Implicit stage (numerical work) $\Rightarrow$ leads to Pole of ζ;
- Order (precision) $\Rightarrow$ star shape on principal sheet;
- A-stability $\Rightarrow$ order star away from imaginary axis.

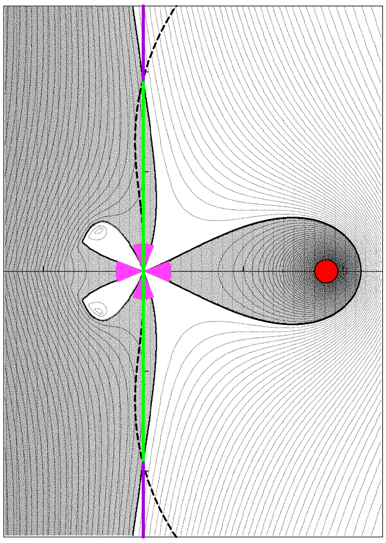
This transforms *numeric properties* (left) to *geometric properties* (right). Order

3 is *not* possible:

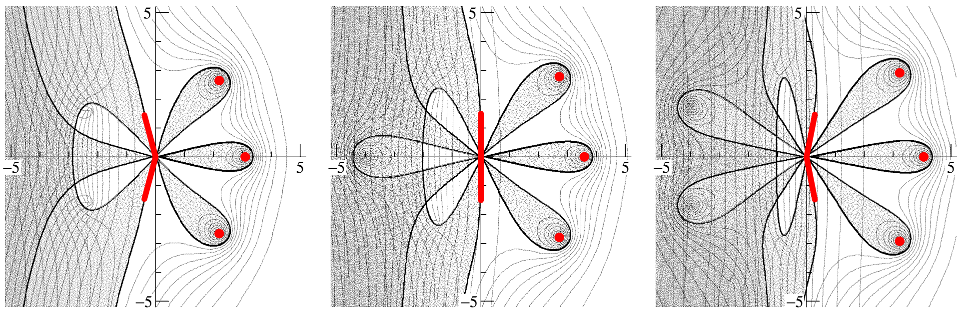
BDF3 method:

$$\frac{11}{6}y_{n+1} - 3y_n + \frac{3}{2}y_{n-1} - \frac{1}{3}y_{n-2} = hf_{n+1}$$

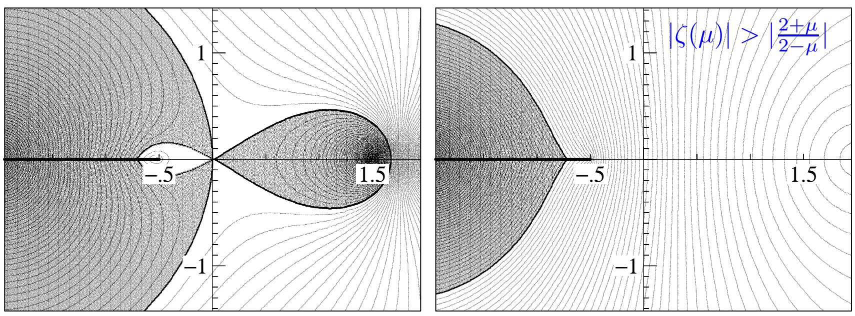
$$\Big(\frac{11}{6} - \mu\Big)\zeta^3 - 3\zeta^2 + \frac{3}{2}\zeta - \frac{1}{3} = 0.$$



The Daniel-Moore Conjecture (A-stab. $\Rightarrow$ $p \le 2s$) is proved similarly:



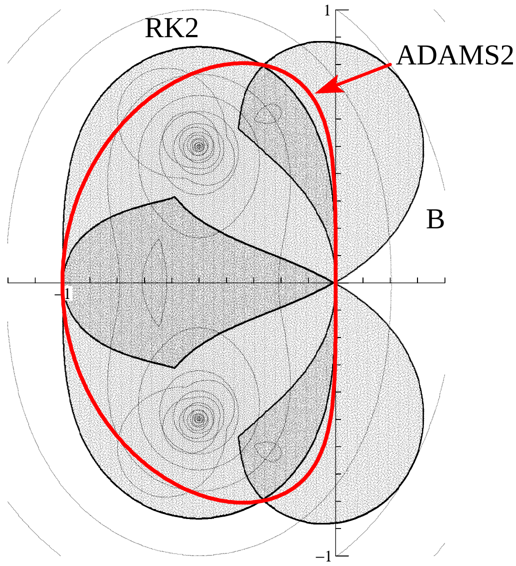
Error constant. In order to prove the *second* part of Dahlquist's theorem (and of the Daniel-Moore conjecture), concerning the smallest error constant, we compare the stability function of our method — not to the exponential function — but to the trapezoidal rule (resp. the diagonal Padé methods):



Jeltsch-Nevanlinna Theorem. The above idea can be extended to *any pair of two methods* and we arrive at another surprising result concerning *scaled* stability domains ("scaled" in the sense to possess the same number of explicit stages per step unit, see [15], [16])

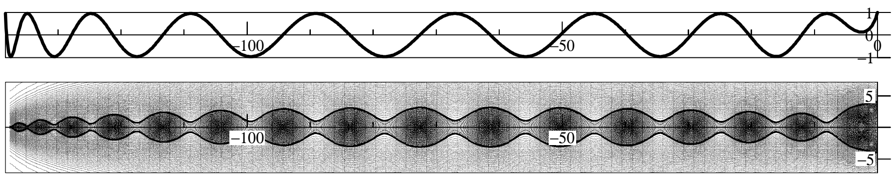
$$S_1^{scal} \not\supset S_2^{scal} \qquad \text{and} \qquad S_1^{scal} \not\subset S_2^{scal}$$

Proof:



This surprising result states that for *every* couple of explicit methods with comparable numerical work there exists always a problem for which one method is more stable than the other and vice-versa.

Stabilized Explicit Methods. *Real* progress, however, is possible, if more information about the position of the eigenvalues of the Jacobian is available. If these eigenvalues are known to be on the real axis, such as in the case of discretized parabolic problems, spectacular progress is possible with the so-called Runge-Kutta-Chebyshev methods. These methods go back, for order 1, to 1960 (see references in [11], second ed. p. 31f) and have been developed for order 2 independently by van der Houwen, Sommeijer and Verwer in Amsterdam, and V.I. Lebedev and A. Medovikov in Moscow. A combination of both approaches led to the ROCK4 algorithm of order 4 of Abdulle [1], which, for $n = 20$, possesses the following stability polynomial and domain



An excellent description of all these methods is given in the book of Hundsdorfer and Verwer [13], Chap. V.

5 Epilogue.

The enthusiasm of all these discoveries had once led the author to present a little story "The Gården of A-stability" in four acts, which Dahlquist remembered still 12 years later (see facsimile in Fig. 5.1). This encourages the author to terminate this exposition with a reproduction of these slides in Fig. 5.2.

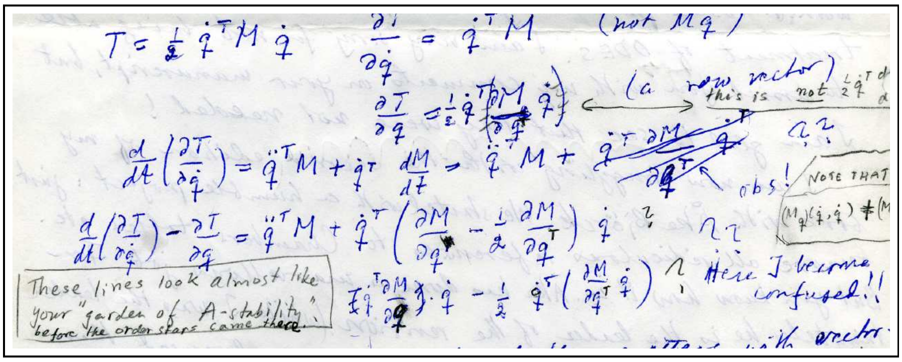


Figure 5.1: From a letter of G. Dahlquist, 30 Sept. 1991)

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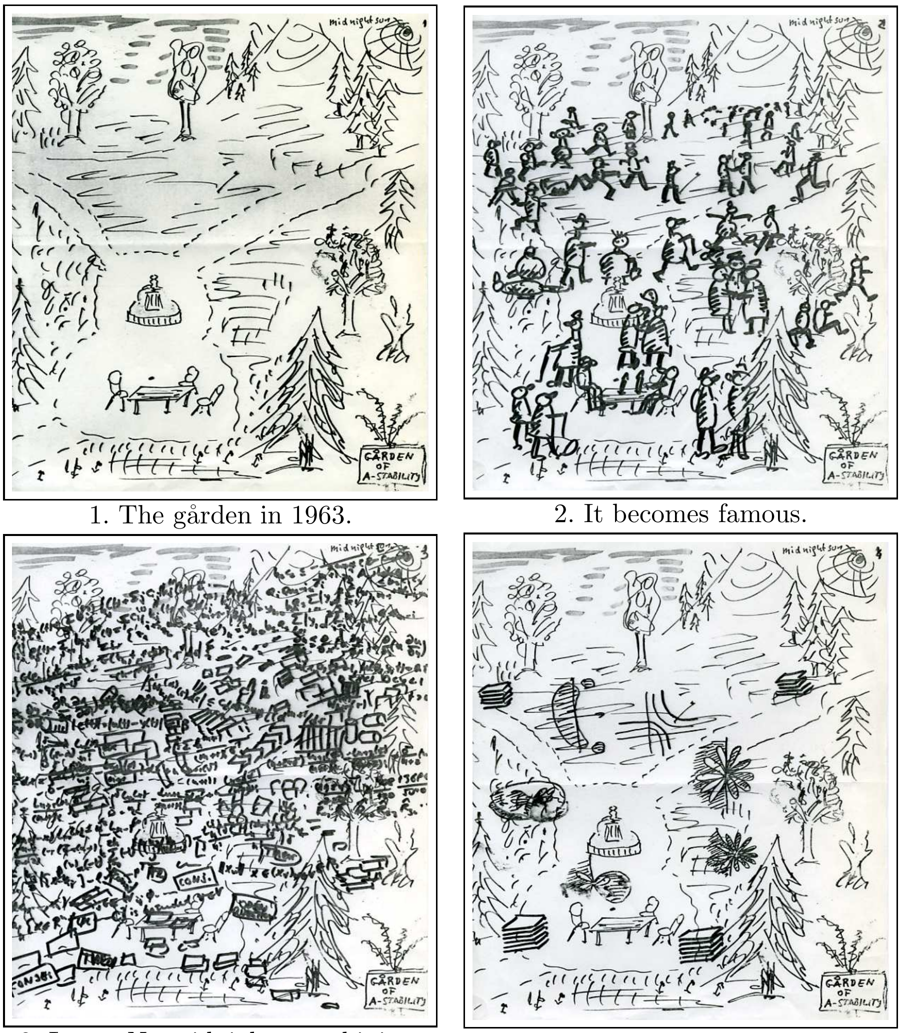

1. The gården in 1963. 2. It becomes famous.

3. Later; No midnight sun shining. 4. Midnight sun is shining again.

Figure 5.2: The *Gården of A-stability* during one and a half decade (slides of the author, presented in Stockholm, May 1979)

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