Numerical Stability of Methods of Lines For Partial Differential Equations

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The method of lines for the numerical treatment of partial differential equations is the technique which consists in using finite differences for the approximation of derivatives with respect to all the independent variables except one, thus obtaining a set or a system of ordinary differential equations. These are then integrated on a digital computer by the use of the well-known numerical methods for such problems.

For initial value type partial differential equations, the names of continuous space and continuous time are used to distinguish methods of lines where the remaining continuous independent variable is either a spatial coordinate x or the time t, respectively.

Our interest in this paper will be restricted to the continuous time methods of lines for initial value problems. In these, one obtains a system of coupled ordinary differential equations which is also of the initial value type.

In addition to the classical implementation of numerical algorithms for the integration of such problems, the recent development of continuous simulation languages, such as CSMP [1] and CSSL [2], provides a means whereby certain of these algorithms are conveniently available as pre-programmed subroutines. This, plus the fact that considerable knowledge about the properties of the numerical integration of initial value problems in ordinary differential equations has been developed in recent years, has prompted a renewed interest in this area.

The first description of methods of lines for the computer solution of partial differential equations seems to be that of Hartree [13], who was interested in the use of mechanical differential analysers. More recently, a concise description of the numerical implementation of continuous-time methods of lines for parabolic equations was given among others by Hicks and Wei [14]. Methods of lines have been one of the main tools in the application of electronic differential analysers (analog and hybrid computers) to the solution of partial differential equations and a considerable literature has been devoted to this subject (see e.g., the references cited in [20]).

It should also be mentioned that several authors have devoted their attention to methods of lines taken in a somewhat different context than that adopted here. In an often referred to paper, Rothe [18] used continuous-space methods of lines strictly as a concept to prove the existence of the solution of certain parabolic equations. The Russians are credited with the coinage of the name of "methods of lines". The reader is referred to the publications of Faddeyeva [7] and Budak [4] in this respect.

A question which has not been well analyzed to date is that of the numerical stability of methods of lines. The prediction of numerical stability is, of course, of great importance in practice, and it is to that specific question that we address ourselves in this paper.

GENERAL FORMULATION

We consider the partial differential equation of the initial/boundary value type:

$$\frac{\partial u}{\partial t} = X(u) \tag{1}$$

where $u = u(x,t)$ is a function of one or several spatial variables x, and of time t, and

$X(\cdot)$ is a partial differential operator involving derivatives with respect to the variable(s) x.

Associated to (1) are a sufficient number of initial and boundary conditions.

We shall, in the ensuing analysis, assume that $X(\cdot)$ is linear. The purpose of this analysis is to derive stability conditions of numerical algorithms used to obtain solutions of (1), and the linearity assumption is equivalent to considering linearized forms of non-linear problems. Such linearized forms are classically used in numerical analysis to describe, in a restricted sense, the behavior of error terms which correctly predict certain numerical instabilities occurring in small regions in space and time.

For simplicity, our notations will be restricted to one-dimensional x spaces, although it must be recognized that all results obtained are easily extended to several dimensional spaces.

Let $\{ x_n = n \cdot \Delta x, \; n = 1,2, \ldots\ldots \; N \}$ be a grid of equidistant points along the x axis (called the solution points), and let $u_n(t)$ be the approximation of $u(x_n,t)$.

The operator $X(\cdot)$ may then be replaced by common finite difference approximations. These are expressed in the general form:

$$\left[X(u) \right]_n \simeq \sum_{\beta} A_{\beta} \, u_{n+\beta} \tag{2}$$

where, under the preceding assumptions, the A_{β} are constant coefficients.

Along the lines $x = x_n$ which are parallel to the time axis, equation (1) is approximated by the system of ordinary differential equations* which is obtained by the use of (2):

$$\frac{du_n}{dt} = \sum_{\beta} A_{\beta} u_{n+\beta} \tag{3}$$

This constitutes an initial value problem which may be integrated numerically by the use of the classical algorithms for systems of ordinary differential equations. With this end in view, we discretize the time t in equal intervals, $t^j = j \cdot \Delta t$, $j = 0, 1, 2, \ldots$ and let u_n^j be the approximation of $u_n(t^j)$.

Use of numerical integration algorithms then yields time-marching procedures by which values of u_n^j are obtained sequentially for $j = 1,2, \ldots$ etc.

We may observe that the analysis of numerical stability in the integration of the partial differential equation (1) consists of analyzing the conditions of numerical stability in the integration of the system of ordinary differential equations (3).

This has two aspects, which are:

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* More specifically, this constitutes a system of difference-differential equations.

(i) To specific classes of partial differential equations will correspond specific properties of the system of equations (3), and

(ii) To specific algorithms for the integration in time of (3) will correspond numerical stability conditions which are specific to those algorithms.

The systematic exploitation of the dual aspects of stability contained in the foregoing observation constitutes an essential aspect of the method of analysis which is developed in the sequel.

STABILITY ANALYSIS

For notation convenience, we introduce the classical space-shift operator E and the time-shift operator z, formally defined by:

$$E \cdot u_n^j = u_{n+1}^j \tag{4}$$

and

$$z \cdot u_n^j = u_n^{j+1} \tag{5}$$

By the use of the operator E, the difference approximation (2) of $X(\cdot)$ may be rewritten in operator notation:

$$\left[X(u) \right]_n \simeq A_\cdot \cdot u_n \; ; \quad A_\cdot \equiv \sum_\beta A_\beta \cdot E^{(\beta)} . \tag{6}$$

such that (3) becomes:

$$\frac{du_n}{dt} = A_\cdot \cdot u_n \tag{7}$$

Similarly, the use of the time-shift operator z affords the expression of integration-in-time numerical algorithms in the convenient general form (see Appendix):

$$u_n^{j+1} = M(\Delta t \cdot A_\cdot, z) \cdot u_n^j \tag{8}$$

The expression of the operator $M(\Delta t \cdot A_\cdot, z)$ contains integer powers of $\Delta t \cdot A_\cdot$, and is independent of z for two-level explicit procedures. It contains a linear term in z for implicit procedures and terms in integer powers of z^{-1} for multi- (more than two) level algorithms.

E. g., the simple Euler rule:

$$u_n^{j+1} = u_n^j + \Delta t \cdot A \cdot u_n^j \tag{9}$$

may be rewritten as (8) with

$$M = 1 + \Delta t \cdot A \cdot \tag{9.a}$$

The first order implicit algorithm

$$u_n^{j+1} = u_n^j + \Delta t \cdot A \cdot u_n^{j+1} \tag{10}$$

yields

$$M = 1 + \Delta t \cdot A \cdot z \tag{10.a}$$

and the "leap frog" three-level predictor method,

$$u^{j+1} = u^{j-1} + 2 \cdot \Delta t \cdot A \cdot u^j \tag{11}$$

yields

$$M = z^{-1} + 2 \cdot \Delta t \cdot A \tag{11.a}$$

To analyze the numerical stability of the procedure (8), we seek, in the classical fashion, trial solutions which are of the form:

$$u_n^j = a^j e^{i\omega x_n} \tag{12}$$

First, we recognize that $e^{i\omega x_n}$ is an eigenfunction of the operator A·, that is:

$$\hat{A} \cdot e^{i\omega x_n} = \hat{A}(\omega)\, e^{i\omega x_n}$$

where $\hat{A}(\omega)$ is a (complex) scalar function, equal to

$$\hat{A}(\omega) = \sum_\beta A_\beta e^{i\omega\beta\Delta x} \tag{13}$$

The scalar function $\hat{A}(\omega)$ is a spectral representation of the operator A· . We therefore call it the <u>spectral function</u> of A.

Because $M(\Delta t \cdot A \cdot, z)$ is a polynomial in $A \cdot$, the functions $e^{i\omega x_n}$ are eigenfunctions of M also. Specifically, we have:

$$M(\Delta t \cdot A, z)\ e^{i\omega x_n} = M(\Delta t \cdot \hat{A}(\omega), z)\ e^{i\omega x_n} \tag{14}$$

where $M(\Delta t \cdot \hat{A}(\omega), z)$ is now an operator in which the space-shift operator E has been eliminated.

Accordingly, substitution of the trial solution (12) into (8) results, after elimination of the common factor $e^{i\omega x_n}$, in the relation between the scalars a^{j+1} and a^j:

$$a^{j+1} = M(\Delta t \cdot \hat{A}(\omega), z)\ a^j \tag{15}$$

A sequence of a^j which is a solution of (15) may be obtained by seeking such solutions which are of the form

$$\frac{a^{j+1}}{a^j} = z \tag{16}$$

where z is now a constant scalar number.

By direct substitution of (16) into (15), we find that this number must be a solution of the characteristic equation (15)', which is:

$$z - M(\Delta t \cdot \hat{A}(\omega), z) = 0 \tag{17}$$

If there exist solutions z of that characteristic equation which are in absolute value larger than unity, then there will exist corresponding sequences a^j which are unbounded for $j \to \infty$, since they are of the form:

$$a^j = a^o \cdot z^{(j)}$$

Hence, we may state the following theorem:

Theorem:

> A necessary condition of numerical stability of the method of lines described by (8) is that all z solutions of the characteristic equation (17) satisfy the condition $|z| \leq 1$ for all values of ω .

This condition is identical to the classical von Neumann condition for difference methods [17], and the eigenvalues z of (17) are equivalent to the amplification factors defined in that context.

STABILITY REGIONS

The analysis is greatly simplified by noting that the characteristic equation (16) may be considered as a transformation by which, to the region $|z| \leq 1$ in the z complex plane, corresponds a region S in the $\Delta t \cdot \hat{A}(\omega)$ complex plane; we call this region S the stability region* of the method of integration in time M utilized, and its boundary is called the stability boundary, S_B.

Figures 1, 2 and 3 depict these regions for the generalized implicit method, for the Runge-Kutta methods of order one to four, and for several predictor/corrector formulae. (The description of these methods in M operator notation is given for reference in the Appendix.)

We note that the function $A(\omega)$ of the parameter ω has a form which depends only on the operator $A\cdot$, that is to say, depends on the equation (1) to be integrated, on the manner in which the operator $X(\cdot)$ is approximated by finite differences, and, implicitly through the A_β coefficients, on the space-discretization step Δx.

As previously remarked, and as will be illustrated by examples, the separate consideration of the spectral function $\hat{A}(\omega)$ (which is equation dependent) and of the stability regions S (which are dependent upon the integration in time M utilized) affords a flexible tool for the analysis of numerical stability.

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* Stability charts for the analysis of numerical integration of systems of ordinary differential equations were first introduced in the 1950's by Gray [3], and by Gurk and Rubinoff [10,11] who restricted their published accounts to a few predictor-corrector formulae. Extension to other explicit methods for ordinary differential equations has been made by Benyon and Hafner [3,12] who were interested mostly in the ordinary differential equations describing the dynamics of aerospace and other mechanical systems.

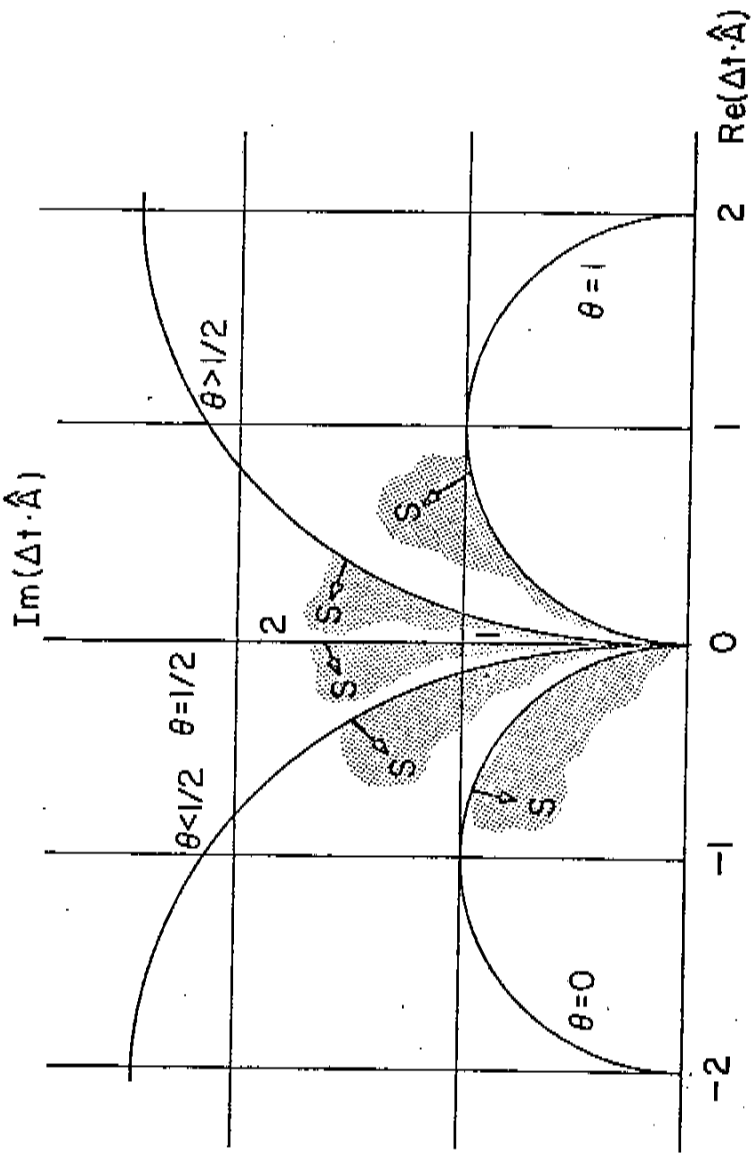

FIGURE 1 – STABILITY REGIONS FOR THE GENERALIZED IMPLICIT METHOD OF INTEGRATION.
(θ VARIABLE FROM 0 TO 1)

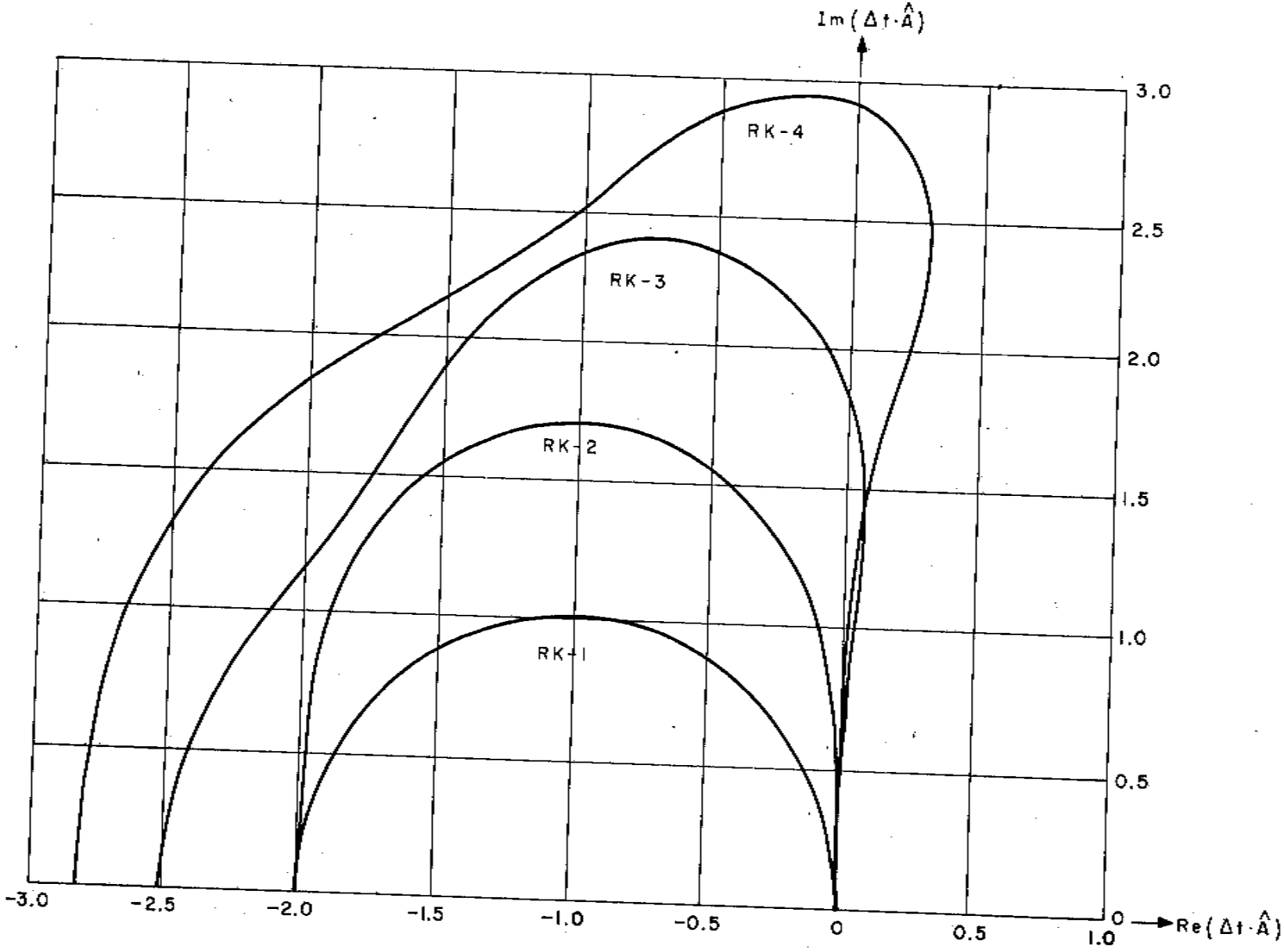

FIGURE 2. STABILITY BOUNDARY FOR RUNGE–KUTTA METHODS OF INTEGRATION IN TIME

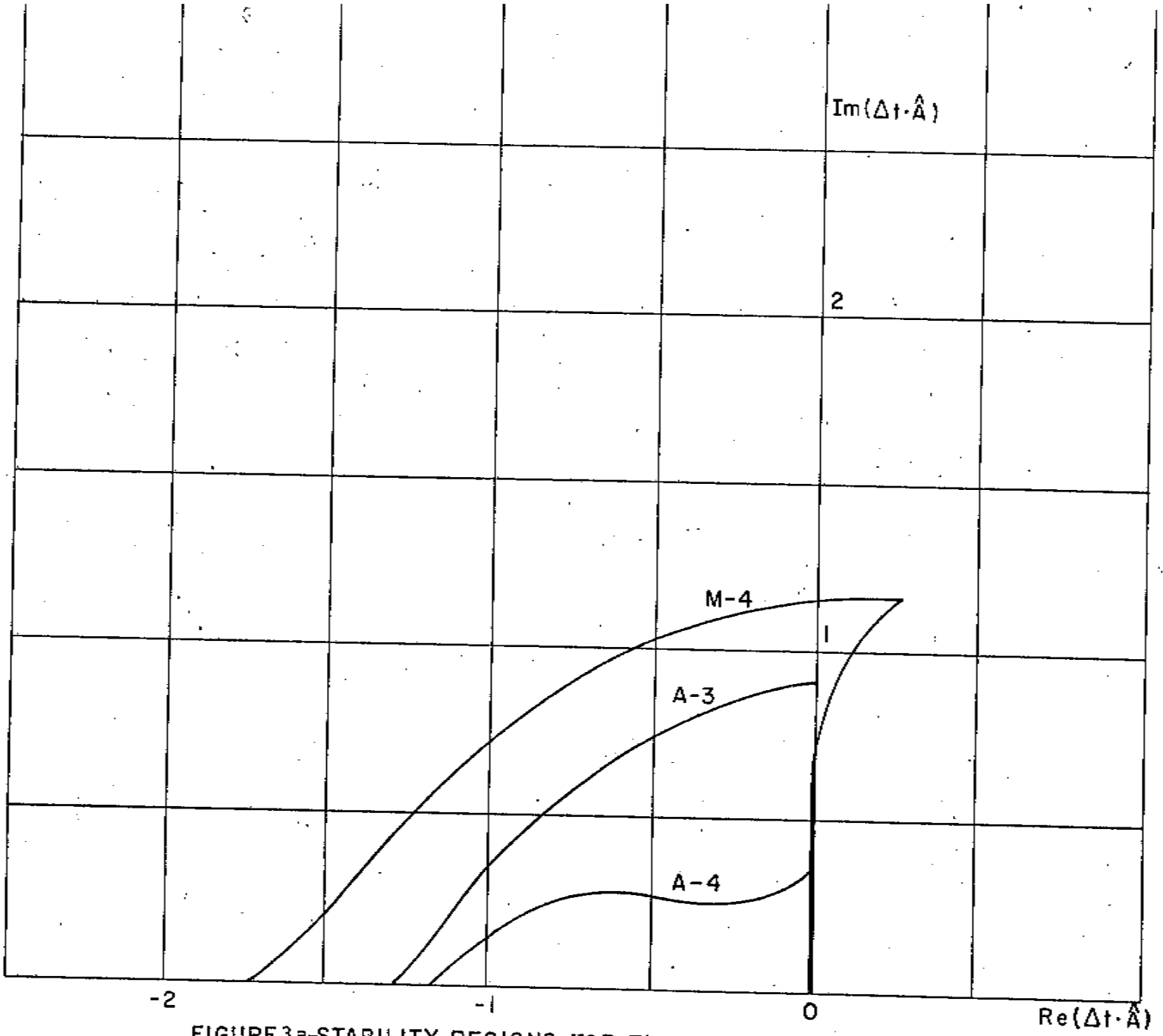

FIGURE 3.a-STABILITY REGIONS FOR THE MILNE FOURTH ORDER AND ADAMS THIRD AND FOURTH ORDER PREDICTOR/CORRECTORS

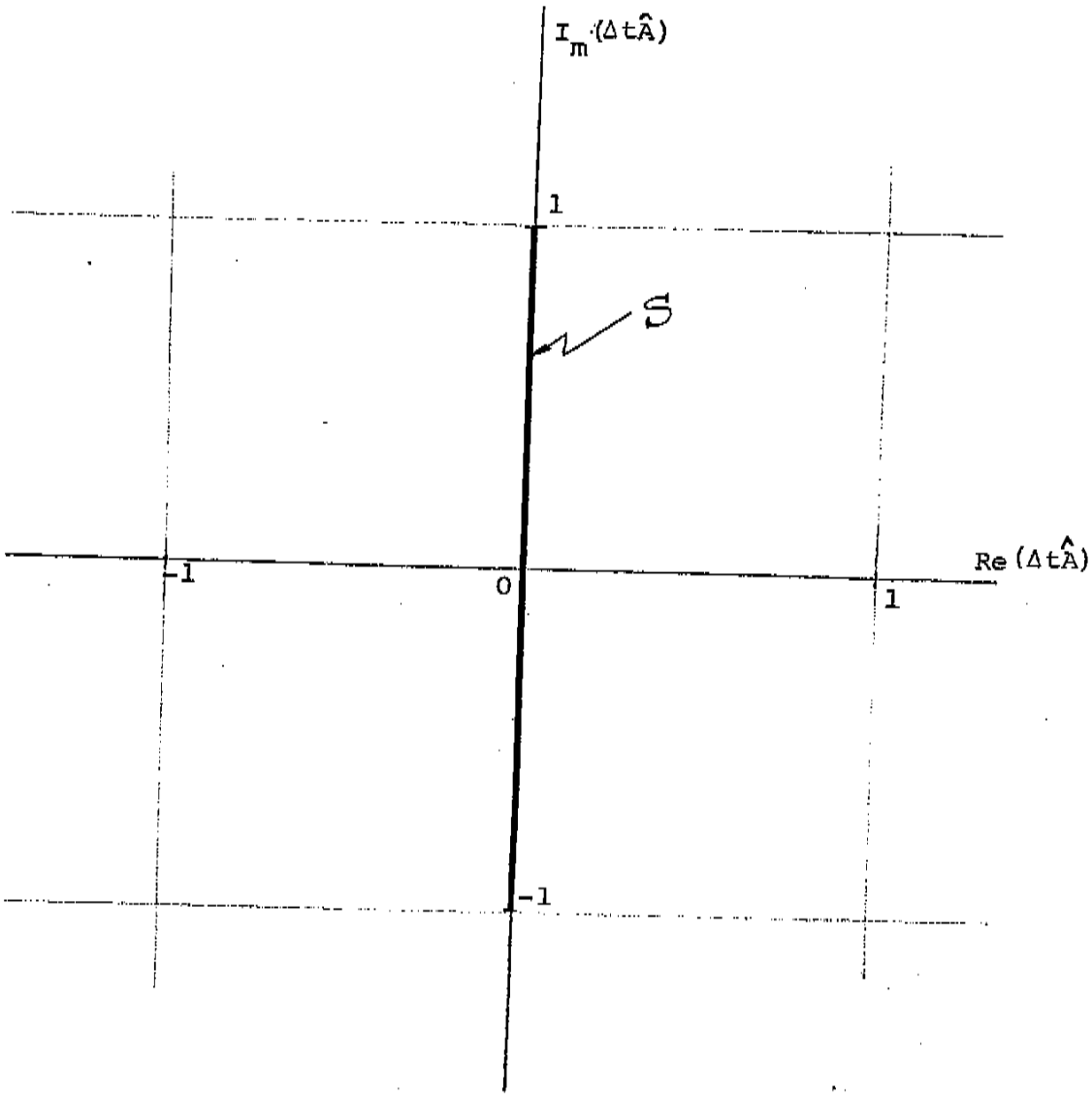

Figure 3.b

Stability Region of the Leapfrog (Predictor) Method of Integration (A-10)
S is limited to the segment (-i,+ i) of the imaginary axis

PARABOLIC EQUATIONS

The simple heat equation

$$\frac{\partial u}{\partial t} = \sigma \frac{\partial^2 u}{\partial x^2} \tag{18}$$

is approximated by central finite differences in space by:

$$\frac{du_n}{dt} = \sigma \left[\frac{u_{n+1} + u_{n-1} - 2u_n}{\Delta x^2} \right] \tag{19}$$

which is of the form (3) with

$$A_{-1} = A_1 = \frac{\sigma}{\Delta x^2} \quad ; \quad A_o = \frac{-2\sigma}{\Delta x^2} \tag{20}$$

The spectral function $\hat{A}(\omega)$ is easily found to be

$$\hat{A}(\omega) = -\frac{2\sigma}{\Delta x^2} (1 - \cos \omega \cdot \Delta x) \tag{21}$$

and is real-negative for all values of ω.

We may note at this point that, with the exception of the "leap-frog" algorithm (11), the stability regions S for most common integration-in-time algorithms M enclose at least a portion of the real-negative axis. The condition of numerical stability for these algorithms is that that portion of the real-negative axis contains (21) for all values of ω. If we call S_R the intersection of the stability boundary S_B with the real-negative axis, the condition of numerical stability may be written as:

$$\left| \Delta t \cdot \hat{A}(\omega) \right|_{max} = \frac{4\sigma \cdot \Delta t}{\Delta x^2} \leq |S_R| \tag{22}$$

E.g., for Euler's method, this leads to the condition:

$$\frac{4.\sigma.\Delta t}{\Delta x^2} \leq |S_R|_{\text{Euler}} = 2$$

or

$$\frac{\sigma.\Delta t}{\Delta x^2} \leq 1/2 \qquad (23)$$

which is the classical stability condition for the explicit difference approximation of the heat equation [17].

The value of $|S_R|$ for other common integration algorithms are summarized in Table 1, together with the corresponding numerical stability conditions for the parabolic difference-differential equation (19).

TABLE 1

Conditions of numerical stability in the integration of the parabolic equation $\frac{\partial u}{\partial t} = \sigma \frac{\partial^2 u}{\partial x^2}$ expressed as the system of ordinary differential equations

$$\frac{du_n}{dt} = \frac{\sigma}{\Delta x^2}\left[u_{n+1} + u_{n-1} - 2u_n\right]$$

and integrated in time by the algorithm M.

Algorithm M			
Name	Equation No. in the text*	$\lvert S_R \rvert$	Stability Condition $\frac{4\,\sigma\cdot\Delta t}{\Delta x^2} \le \lvert S_R \rvert$
Euler	(9), (A-3)	2	$\frac{\sigma\cdot\Delta t}{\Delta x^2} \le \frac{1}{2}$
Leapfrog (Richardson 1910) Three Level Predictor	(11)	0	Always Unstable
Generalized Implicit	(A-3)	$\frac{2}{1-2\theta}$ for $\theta < \frac{1}{2}$ ∞ for $\theta \ge \frac{1}{2}$	$\frac{\sigma\cdot\Delta t}{\Delta x^2} \le \frac{1}{2(1-2\theta)}$ for $\theta < \frac{1}{2}$ Always stable for $\theta \ge \frac{1}{2}$
Runge-Kutta-2	(A-6)	2	$\frac{\sigma\cdot\Delta t}{\Delta x^2} \le \frac{1}{2}$
Runge-Kutta-4	(A-5),(A-6)	2.9	$\frac{\sigma\cdot\Delta t}{\Delta x^2} \le .73$
Milne 4th Order Predictor/ Corrector	(A-7)	1.2	$\frac{\sigma\cdot\Delta t}{\Delta x^2} \le .3$
Adams - 3rd Order Predictor/ Corrector	(A-8)	1.7	$\frac{\sigma\cdot\Delta t}{\Delta x^2} \le .425$
Adams - 4th Order Predictor/ Corrector	(A-9)	1.26	$\frac{\sigma\cdot\Delta t}{\Delta x^2} \le .315$

* (A-) refers to equation numbers in the Appendix.

HYPERBOLIC EQUATIONS

The general hyperbolic system,

$$\frac{\partial U}{\partial t} + f\frac{\partial U}{\partial x} = 0 \tag{24}$$

where U is an m-vector of functions of x and t, and f an (m x m) matrix having real eigenvalues and distinct eigenvectors, may be transformed by a similarity transformation into the m equations:

$$\frac{\partial u_i}{\partial t} + C_i\frac{\partial u_i}{\partial x} = 0 \tag{25}$$

where the C_i are the characteristic values of f and have the dimension of a velocity $\frac{dx}{dt}$. The treatment of (24) by the method of lines is equivalent, in the linear case, to the independent treatment of the m equations (25). And the numerical stability properties of the first may be derived by analyzing the stability of the latter separately for each i. Therefore, to analyze the numerical stability of methods of lines applied to (24), we shall analyze the numerical stability of:

$$\frac{\partial u}{\partial t} + C\frac{\partial u}{\partial x} = 0 \tag{26}$$

where C takes on the value of all the characteristic values of f.

Central Differences

The simple central difference approximation of $\frac{\partial u}{\partial x}$ is:

$$\left[\frac{\partial u}{\partial x}\right]_n \simeq \frac{u_{n+1} - u_{n-1}}{2 \cdot \Delta x} \tag{27}$$

so that (26) may be approximated by:

$$\frac{du_n}{dt} = - \frac{C}{2 \cdot \Delta x} \left[u_{n+1} - u_{n-1} \right] \tag{28}$$

This is of the form (3) with $A_1 = -A_{-1} = - \frac{C}{2 \cdot \Delta x}$.

The spectral function of the right-hand side of (28) is found to be

$$A(\omega) = \frac{-iC}{\Delta x} \cdot \sin (\omega \cdot \Delta x) \tag{29}$$

and is pure-imaginary for all values of ω .

As we may see, in Figs. 1, 2 and 3, several of the usual integration-in-time algorithms have stability regions S which do not enclose any portion of the imaginary axis. If these were applied to the integration of (28), they would lead to completely unstable procedures. This includes, among others, the first order explicit or Euler method, the Runge-Kutta-2 method and the generalized implicit method (A-3) for $\theta < \frac{1}{2}$.

On the other hand, the leap-frog method for which the stability region S is restricted to the segment of the imaginary axis [-i,+i] (fig.3.b), and which is always unstable for parabolic equations, is stable here, provided that

$$\left| i \frac{C \cdot \Delta t}{\Delta x} \cdot \sin (\omega \cdot \Delta x) \right| \leq |i| \quad \text{for all values of } \omega$$

i.e.,

$$\left| \frac{C \cdot \Delta t}{\Delta x} \right| \leq 1 \tag{30}$$

This is the well-known Courant-Friedrich-Lewy condition of stability for this procedure [5]

If we call S_I the intersection of the stability boundary S_B of an integration algorithm M with the imaginary axis, the numerical stability condition for the hyperbolic difference-differential equation (28) may be expressed as:

$$\left| \Delta t \cdot A(\omega) \right|_{max} = \left| \frac{C \cdot \Delta t}{\Delta x} \sin(\omega \cdot \Delta x) \right|_{max} = \left| \frac{C \cdot \Delta t}{\Delta x} \right| \leq \left| S_I \right| \tag{31}$$

The value of $\left| S_I \right|$ for common integration algorithms is summarized in Table 2, together with the corresponding numerical stability condition for the hyperbolic difference-differential equation (28).

TABLE 2

Conditions of numerical stability in the integration of the hyperbolic equation, $\frac{\partial U}{\partial t} + f \cdot \frac{\partial U}{\partial x} = 0$, expressed as the system of ordinary differential equations, $\frac{dU_n}{dt} + f\left[\frac{U_{n+1} - U_{n-1}}{2 \cdot \Delta x}\right] = 0$ and integrated in time by the algorithm M.

Algorithm M			
Name	Equation No. in the Text	$\lvert S_I \rvert$	Stability Condition $\left\lvert \frac{C \cdot \Delta t}{\Delta x} \right\rvert \leq \lvert S_I \rvert$ where C is the eigenvalue of f of highest absolute value
Euler	(9), (A-3)	0	Always Unstable
Leapfrog Three-Level Predictor	(11)	1	$\left\lvert \frac{C \cdot \Delta t}{\Delta x} \right\rvert \leq 1$
Generalized Implicit	(A-3)	0 for $\theta < \frac{1}{2}$ ∞ for $\theta \geq \frac{1}{2}$	Unstable for $\theta < \frac{1}{2}$ Stable for $\theta \geq \frac{1}{2}$
Runge Kutta-2	(A-6)	0	Always Unstable
Runge Kutta-4	(A-5), (A-6)	2.85	$\left\lvert \frac{C \cdot \Delta t}{\Delta x} \right\rvert \leq 2.85$
Milne 4th Order Predictor/ Corrector	(A-7)	.37	$\left\lvert \frac{C \cdot \Delta t}{\Delta x} \right\rvert \leq .37$
Adams 3rd Order Predictor/ Corrector	(A-8)	1.2	$\left\lvert \frac{C \cdot \Delta t}{\Delta x} \right\rvert \leq 1.2$
Adams 4th Order Predictor/ Corrector	(A-9)	.9	$\left\lvert \frac{C \cdot \Delta t}{\Delta x} \right\rvert \leq .9$

EXTENSION TO OTHER CASES: A Heuristic Classification of Partial Differential Equations

For our purpose, we may categorize partial differential equations of the initial value type into classes which reflect the nature of the spectral function $\hat{A}(\omega)$ of their difference approximation.* Whenever the $\hat{A}(\omega)$ are real negative, the numerical stability properties will be analogous to those of the parabolic equation (18). In this category, we find the equation:

$$\frac{\partial u}{\partial t} = (-1)^{\frac{r}{2}+1} \frac{\partial^r u}{\partial x^r} \tag{32}$$

where r is any even positive integer.

Whenever the $\hat{A}(\omega)$ are pure imaginary, the numerical stability properties will be analogous to those of the hyperbolic equation (24). Here we find the equation:

$$\frac{\partial u}{\partial t} = \frac{\partial^r u}{\partial x^r} \tag{33}$$

where r is an odd positive integer, and the beam vibration equation:

$$\frac{\partial^2 u}{\partial t^2} + K^2 \frac{\partial^4 u}{\partial x^4} = 0 \tag{34}$$

which may be transformed into a system of equations of the first order in time, for which the $\hat{A}(\omega)$ are found to be indeed pure imaginary. (The latter extention requires a generalization of the concepts presented in this paper which are based on matrix calculations. This will not be pursued here but may be found in [19].)

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*As noted, the nature of the $\hat{A}(\omega)$ depends on the way in which the finite difference approximation of $X(\cdot)$ is derived. We shall assume here that all such approximations are of the central difference type.

Denote by $\hat{X}(\omega)$ the spectral function of the operator $X(\cdot)$, defined by:

$$\hat{X}(\omega) \triangleq X(e^{i\omega x}) / e^{i\omega x}$$

In general, central difference approximations of $X(\cdot)$ have spectral functions $\hat{A}(\omega)$ which are real/imaginary/complex whenever $\hat{X}(\omega)$ is real/imaginary/complex, so that the properties of $\hat{A}(\omega)$ are in fact properties which are specific to the original equation (1) itself.

We may note that, although this equation is generally classified as parabolic in the classical sense (e.g., ref. [6]), its numerical stability characteristics make it more akin to hyperbolic equations in that respect.

When the $\hat{A}(\omega)$ are complex (we assume that they are restricted to the left side of the complex plane), the numerical stability properties will vary continuously from those of the hyperbolic equation (23) to those of the parabolic equation (18), depending upon the ratio of the imaginary and real part of $\hat{A}(\omega)$. At any rate, the use of the stability regions affords a direct derivation of those properties.

This may be illustrated by consideration of the transport-diffusion equation with linear decay term:

$$\frac{\partial u}{\partial t} + C \frac{\partial u}{\partial x} = \sigma \frac{\partial^2 u}{\partial x^2} - gu \tag{35}$$

where C, σ and g are positive constants.

If the central difference approximations (25) and (19) are used for the first and second x-derivatives, the spectral function $\hat{A}(\omega)$ is:

$$\hat{A}(\omega) \equiv -\left[\frac{2\sigma}{\Delta x^2} (1 - \cos \omega \cdot \Delta x) + g \right] - \frac{iC}{\Delta x} (\sin \omega \cdot \Delta x) \tag{36}$$

which is the equation of the ellipse depicted in fig. 4.

We may see, for instance, that the one-half implicit integration (Crank Nicolson) algorithm:

$$M(\Delta t F, z) = 1 + \frac{\Delta t}{2} (\Delta t \cdot F + \Delta t \cdot F \cdot z) \tag{37}$$

is always stable for that equation, while fig. 5.a depicts several combinations of the parameters $C, \sigma, g, \Delta x$ and Δt which are stable when the Runge-Kutta-4 integration algorithm is applied. Similarly, fig. 5.b depicts several combinations of these parameters which yield numerically unstable procedures when integrated by Runge-Kutta-4.

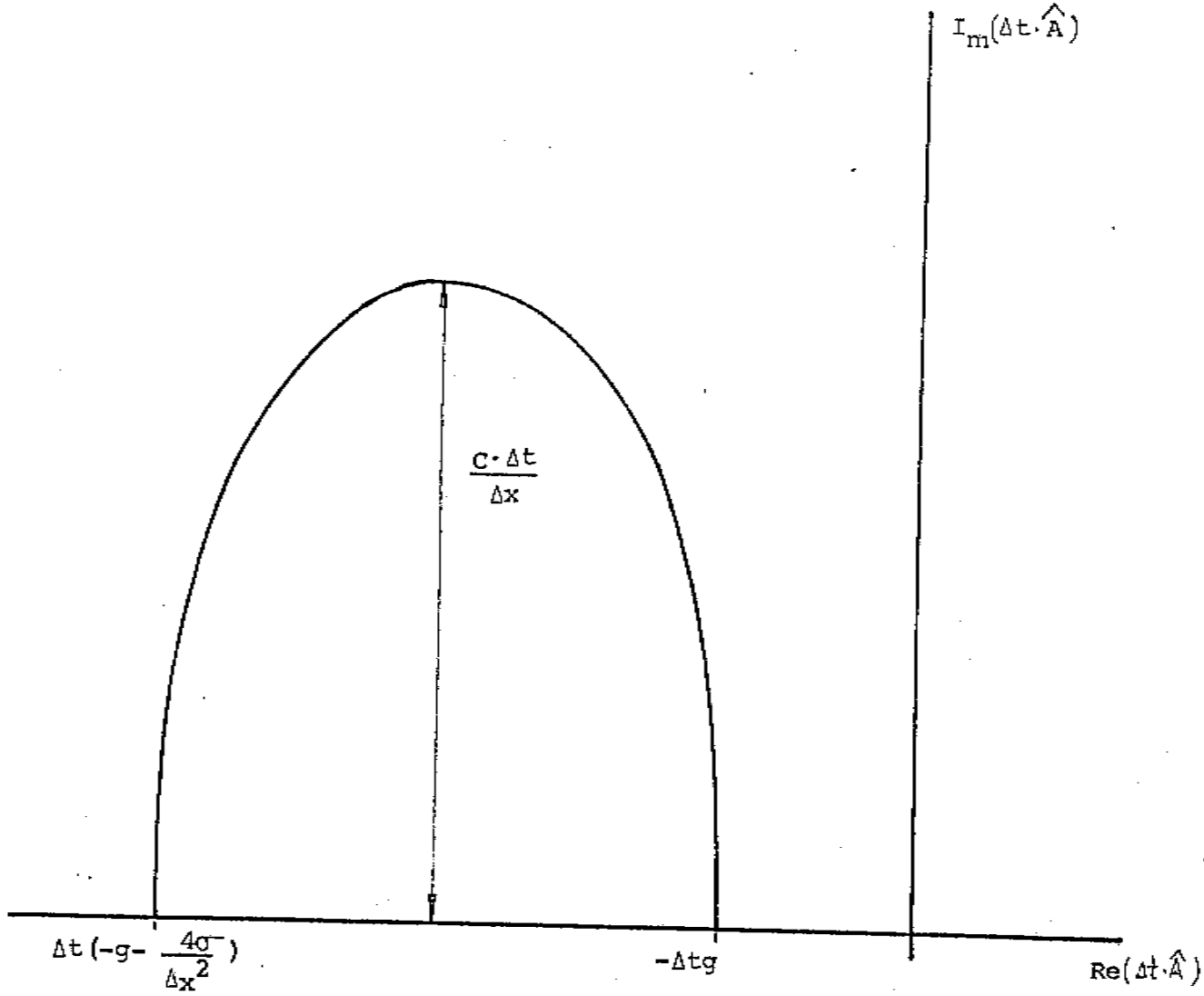

Figure 4 - The Spectral Function $\hat{A}(\omega)$
for the Transport-Diffusion Equation (35)

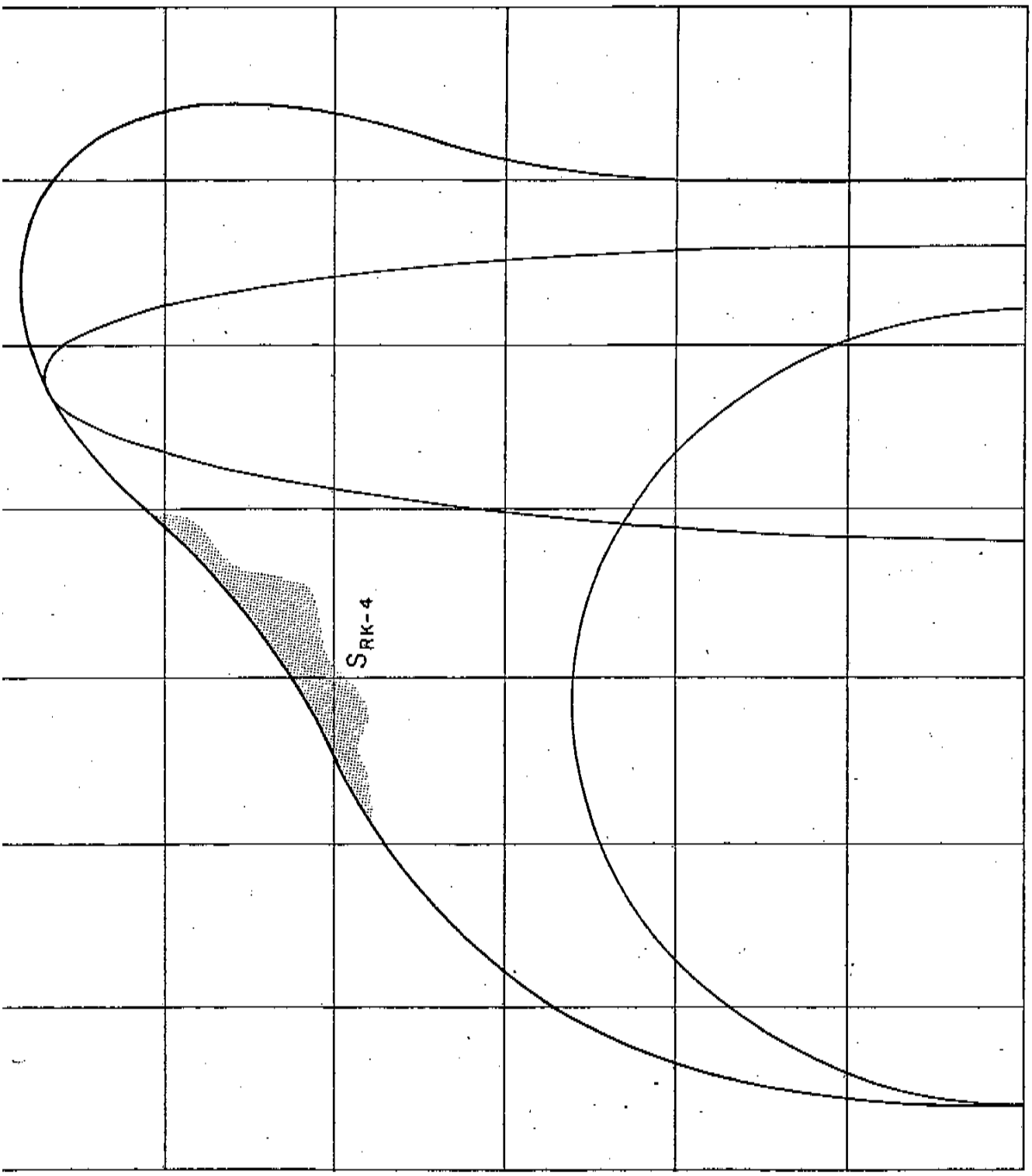

FIGURE. 5.0 — EXAMPLES OF LIMITING STABLE CASES FOR THE INTEGRATION OF THE TRANSPORT-DIFFUSION EQUATION (35) BY THE RUNGE KUTTA-4 METHOD.

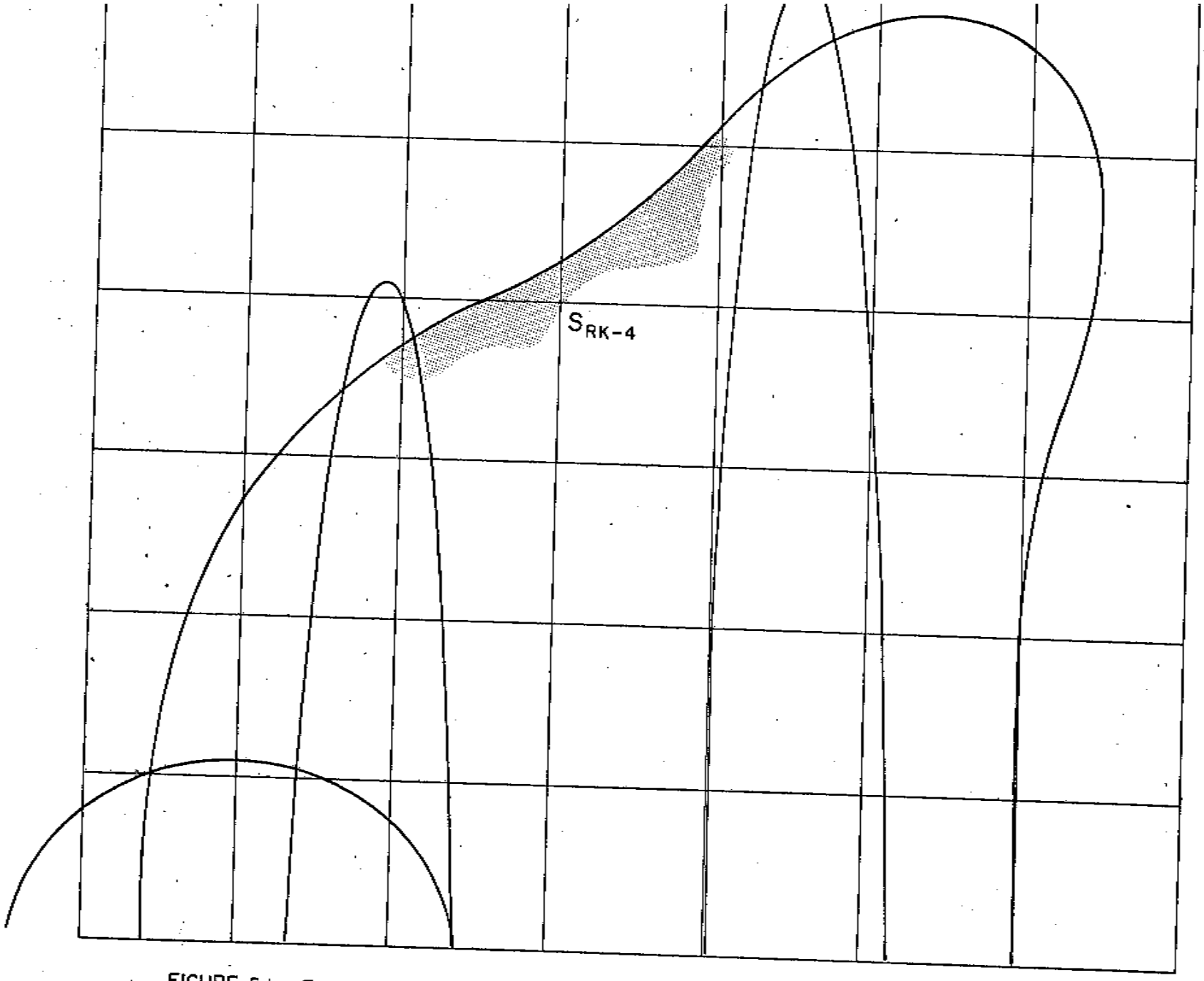

FIGURE 5.b.– EXAMPLE OF UNSTABLE CASES FOR THE INTEGRATION OF THE TRANSPORT – DIFFUSION EQUATION (35) BY THE RUNGE KUTTA – 4 METHOD

APPENDIX

OPERATOR NOTATION FOR COMMON NUMERICAL INTEGRATION ALGORITHMS FOR SYSTEMS OF ORDINARY DIFFERENTIAL EQUATIONS

Common numerical integration algorithms for the system of ordinary differential equations

$$\frac{dY}{dt} = F(Y) \tag{A.1}$$

may be written in general operator notation:

$$Y^{j+1} = M \cdot Y^j \tag{A.2}$$

This notation has been used by previous authors for explicit, two-level methods. (See, e.g., Lapidus [15] page 122, and ref. [8]). For such methods, $M = M(\Delta t \cdot F)$. Our introduction of the operator z into M allows this same notation to be extended to multi-level and to implicit algorithms. The simple generalized implicit formula:

$$Y^{j+1} = Y^j + \Delta t\left[\theta F(Y^{j+1}) + (1-\theta)F(Y^j)\right] \tag{A.3}$$

may be observed to be identical to (A.2), with

$$M = 1+\theta \cdot \Delta t\, F \cdot z + (1-\theta)\cdot \Delta t \cdot F \tag{A.4}$$

For $\theta = 0$, this reduces to the simple Euler rule (9) while for $\theta = 1$, it becomes the first order implicit algorithm (10); for $\theta = \frac{1}{2}$, this is known as the Crank-Nicolson algorithm [17].

The classical Runge-Kutta-4 method is:

$$Y^{j+1} = Y^j + \frac{1}{6}\left[K_1 + 2K_2 + 2K_3 + K_4\right] \qquad \text{(a)}$$

where:

$$\left.\begin{aligned} K_1 &= \Delta t \cdot F(Y^j) \\ K_2 &= \Delta t \cdot F(Y^j + K_{1/2}) \\ K_3 &= \Delta t \cdot F(Y^j + K_{2/2}) \\ K_4 &= \Delta t \cdot F(Y^j + K_3) \end{aligned}\right\} \qquad \text{(b)} \tag{A.5}$$

From this, we may write successively:

$$K_2 = \Delta t \cdot F \left[\left(1 + \frac{\Delta t \cdot F}{2}\right) \cdot Y^j \right]$$

$$K_3 = \Delta t\, F \left[\left(1 + \tfrac{1}{2} \Delta t\, F \left(1 + \frac{\Delta t \cdot F}{2}\right)\right) Y^j \right]$$

$$= \left[\Delta t \cdot F + \frac{(\Delta t\, F)^2}{2} + \frac{(\Delta t\, F)^3}{4} \right] \cdot Y^j$$

$$K_4 = \Delta t\, F \left[\left(1 + (\Delta t \cdot F + \frac{(\Delta t\, F)^2}{2} + \frac{(\Delta t\, F)^3}{4}\right) Y^j \right]$$

$$= \left[\Delta t\, F + \Delta t^2 F^2 + \frac{(\Delta t \cdot F)^3}{2} + \frac{(\Delta t \cdot F)^4}{4} \right] \cdot Y^j$$

Upon substitution in (A.5.a), we find*:

$$Y^{j+1} = \left[1 + \Delta t\, F + \frac{(\Delta t\, F)^2}{2} + \frac{(\Delta t \cdot F)^3}{6} + \frac{(\Delta t \cdot F)^4}{24} \right] \cdot Y^j$$

$$= M \cdot Y^j$$

where, as we may observe:

$$M = \sum_{r=0}^{4} \frac{(\Delta t \cdot F)^r}{r!} \qquad (A.6)$$

And, generally, classical Runge-Kutta methods of order n may be written in the operator notation (A.6) with the upper limit of the summation equal to n.

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* Note the non-accidental similarity with the five first terms of a Taylor Series.

As an example of predictor-corrector methods, the fourth order Milne algorithm:

$$\begin{cases} \text{(Predictor)} \\ Y_P^{j+1} = Y_C^{j-1} + \frac{\Delta t}{3}\left(8F(Y_C^j) - 5F(Y_C^{j-1}) + 4F(Y_C^{j-2}) - F(Y_C^{j-3})\right) \\ \text{(Corrector)} \\ Y_C^{j+1} = \frac{1}{8}(Y_C^j + 7Y_C^{j-1}) + \frac{\Delta t}{192}\left(65F(Y_P^{j+1}) + 243F(Y_C^j) + 51F(Y_C^{j-1}) + F(Y_C^{j-2})\right) \end{cases} \tag{A.7}$$

may be written by substitutions similar to the above, as (A.2), with:

$$M = \frac{(1+7\cdot z^{-1})}{8} + \frac{(243+116z^{-1}+z^{-2})}{192}\cdot\Delta t\cdot F + \frac{(98-5z^{-1}+4z^{-2}-z^{-3})}{576}(\Delta t\cdot F)^2$$

The Adams predictor/corrector methods of order 3 and 4, for which the stability regions are shown in fig. 3.a, are, respectively - (see e.g., [15] page 182):

$$\begin{cases} Y_P^{j+1} = Y_C^j + \frac{\Delta t}{12}\left[23F(Y_C^j) - 16F(Y_C^{j-1}) + 5F(Y_C^{j-2})\right] \\ Y_C^{j+1} = Y_C^j + \frac{\Delta t}{12}\left[5F(Y_P^{j+1}) + 8F(Y_C^j) - F(Y_C^{j-1})\right] \end{cases} \tag{A.8}$$

and

$$\begin{cases} Y_P^{j+1} = Y_C^j + \frac{\Delta t}{24}\left[55F(Y_C^j) - 59F(Y_C^{j-1}) + 37F(Y_C^{j-2}) - 9F(Y_C^{j-3})\right] \\ Y_C^{j+1} = Y_C^j + \frac{\Delta t}{24}\left[9F(Y_P^{j+1}) + 19F(Y_C^j) - 5F(Y_C^{j-1}) + F(Y_C^{j-2})\right] \end{cases} \tag{A.9}$$

(Their re-writing in operator notation is left to the interested reader.)

References

1 Anon., "System 360/CSMP (Continuous System Modeling Program), User's Manual (1969), IBM, White Plains, New York 10601.

2 Anon., "CSSL II (Continuous Systems Simulation Language)", User's Reference Manual, December 1968, Spectrodata, Inc., Los Angeles, Cal. 90045.

3 Benyon, P., "A Review of Numerical Methods for Digital Simulation", SIMULATION, Vol. 11, No. 5, November 1968.

4 Budak, B.M., "The Method of Straight Lines for Certain Boundary Value Problems of the Parabolic Type", Z.V.M. 1(1961) 1105-1112- Orig., C.M.M.P. 1(1962-63) 1284-1291 - Translation.

5 Courant, R., Friedrichs, K.O., and Lewy, H., "Uber die Partiellen Differenzengleichungen der Mathematischen Physik", Math. Ann., Vol. 100, p. 32 (1928).

6 S. H. Crandall and W. C. Royster, "Numerical Treatment of a Fourth Order Parabolic Partial Differential Equation", J. of ACM, Vol. 1: pp. 111-118, 1954.

7 V. N. Faddeyeva, Trans. into English from Tr. Mat. Inst. Akad Nauk SSR (Moscow) v. 28, 1949 p. 73-103, "The Method of Straight Lines in the Application to Certain Boundary Problems".

8 Fowler, M.E. and Warten, R.M., "A Numerical Integration Technique for ODE's with Widely Separated Eigenvalues", IBM Journal of Research and Development, Vol. 11, No. 5, September 1967.

9 H. J. Gray, Jr., "Numerical Methods in Digital Real Time Simulation", Quarterly App. Math., Vol. XII, No. 2, July 1954, pp. 133-140.

10 Gurk, H. M. and Rubinoff, M., "Numerical Solution of Differential Equations", Proc. Eastern Joint Computer Conference, Philadelphia, Pa., December 8-10, 1954, pp. 58-64.

11 Gurk, H. M., "The Use of Stability Charts in the Synthesis of Numerical Quadrature Formulae", Quart. Appl. Math., Vol. 13, April 1955, pp. 73-78.

12 Hafner, P. A., "Stability Charts of Various Numerical Methods Used for Solving Systems of Ordinary Differential Equations", Weapons Research Establishment, Australia, Tech. Note WSD 112, November 1969.

13 Hartree, D. R., and Womersley, J. R., "A Method for the Numerical or Mechanical Solution of Certain Partial Differential Equations", Proc. Roy. Soc., Vol. 161, 1937, p. 353.

14. Hicks, J. S. and Wei, J., "Numerical Solution of Parabolic Partial Differential Equations with Two-Point Boundary Conditions by Use of the Method of Lines", Journal of the ACM, Vol. 14, No. 3, July 1967, pp. 549 ff.

15 Lapidus, L. and Seinfeld, J. H., "Numerical Solution of Ordinary Differential Equations", Academic Press, New York, 1971.

16 O'Brien, G., Hyman, M.A. and Kaplan, S., "A Study of the Numerical Solution of Partial Differential Equations", J. of Math. and Physics, pp. 223 ff.

17 Richtmyer, R.D., and Morton, R. W., "Difference Methods for Initial Value Problems", Interscience Publishers, Inc., New York, 1967, (405 pp.)

18 Rothe, E., "Zweidinentionale Parabolische Randwertaufgaben als Grenzfall Eindimensionaler Randwertaufgaben", Math. Annal. Bd., 102, Heft 4-5, (1929), pp. 650-670.

19 Vichnevetsky, R.,"Numerical Stability of Methods of Lines for the Beam Vibrations Equation", Report #TR 71-18, Electronic Associates, Inc., West Long Branch, N. J., April 1971.

20 Vichnevetsky, R., "State of the Art in Hybrid Methods for Partial Differential Equations", Proceedings, AICA-IFIP International Conference on Hybrid Computation, Munich, Germany, August 31 - September 4, 1970. Publisher, European Academic Press, Brussels.