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ON THE NUMERICAL SOLUTION OF PARTIAL DIFFERENTIAL EQUATIONS OF PARABOLIC TYPE

WORK DONE BY:

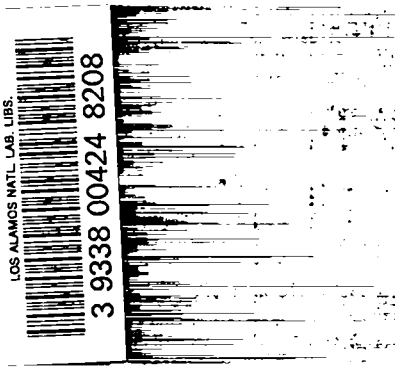
J. vonNeumann
R. D. Richtmyer

REPORT WRITTEN BY:

J. vonNeumann
R. D. Richtmyer

ABSTRACT

A method is described for solution of parabolic differential equations by calculating routines involving stepwise integration in both variables. The main features of the method arise from manipulations introduced to avoid instabilities that generally appear when partial differential equations are converted into difference equations.



ON THE NUMERICAL SOLUTION OF PARTIAL DIFFERENTIAL EQUATIONS OF PARABOLIC TYPE

I. THE EQUATION. The equation

$$(1)\quad \frac{\partial F}{\partial t} = p\,\frac{\partial}{\partial y}\left(q\,\frac{\partial F}{\partial y}\right) + G,$$

where t and y are independent variables, F is the dependent variable and p,q,G are given, smooth functions of t,y and F, is in essence the heat flow equation for a system in which only one space coordinate enters (e.g. by reason of symmetry), in which the thermal conductivity and the specific heat capacity depend on time, position and temperature, and with a distributed heat production at a rate also dependent on time, position and temperature.

If $pq > 0$ (which will be henceforth assumed), we have the well known stability property of parabolic equations, namely that a solution free of sinularities at one time t is free of singularities at all later times.

This report concerns numerical methods of solving (1) by integration procedures which are stepwise in both independent variables. It is clear in principle that if F is known at time t for all y in a certain domain and suitable boundary conditions are applied at the boundaries of the domain, equation (1) then permits determination of F at a slightly later time $t + \Delta t$ and that this process can be repeated. That the establishment of satisfactory calculating routines for doing this is not a trivial problem will be apparent from Section II below.

II. THE EXPLICIT DIFFERENCE SYSTEM. Let us choose a rectangular mesh of points (y_ℓ, t^n), where $\ell = 0,1,2,\cdots$; $n = 0,1,2,\cdots$, in the y-t plane. Without loss of generality, we may assume that the spacing of the points is uniform in both directions, because the variables y,t can be subject to transformations without departing from the assumed form of (1). The actual distribution of mesh points, before this transformation, may have been fixed by considerations of desired accuracy, rapidity of variation of p,q and G with y and t, and perhaps other calculating routines in an overall physical problem of which equation (1) is only a part. The spacings will be denoted by Δt and Δy. The value of any function, say $F(y,t)$, at mesh point (y_ℓ, t^n) will be de-

noted by F_ℓ^n for brevity. Similarly $q_{\ell+\frac{1}{2}}^n$ denotes the value of q at a point midway between (y_ℓ, t^n) and $(y_{\ell+1}, t^n)$; equivalently, to the degree of approximation we shall use, $q_{\ell+\frac{1}{2}}^n$ is the mean of q_ℓ^n and $q_{\ell+1}^n$.

A system of difference equations approximating to (1) is

$$(2)\quad \frac{1}{\Delta t} F_\ell^{n+1} = \frac{1}{\Delta t} F_\ell^n + p_\ell^n \frac{q_{\ell+\frac{1}{2}}^n \left(F_{\ell+1}^n - F_\ell^n\right) - q_{\ell-\frac{1}{2}}^n \left(F_\ell^n - F_{\ell-1}^n\right)}{(\Delta y)^2} + G_\ell^n .$$

The conditions for stability of this system has been discussed by one of us[1]. Although the differential equation is stable in the sense that small irregularities introduced at one time become reduced as time goes on, unless new irregularities are introduced by the "heat production" term G, the difference equations may be unstable; that is, under some circumstances irregularities may be amplified and grow without limit as time goes on; a solution of (2) does not in general approach a solution of (1) as the mesh is made finer and finer unless a certain restriction (equation (3) below) is applied to the relation between Δy and Δt at each stage of the limiting process.

The argument may be summarized as follows: For a sufficiently fine mesh we may treat p, q and G as constant over a region that is small but nevertheless contains many mesh points. If F at a given time t is expanded in a Fourier series in y, we may regard F(y,t) as a superposition of functions, each depending on y through a factor $e^{i\beta y}$, where β is real, and on t through a factor $e^{\alpha t}$, where α (depending on β) may be complex[2]. The relation between α and β is found by substituting such a function into (2) and cancelling out common factors. It is

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(1) Lectures (unpublished) delivered by J. vonNeumann at Los Alamos in February, 1947.

(2) It is, of course, the real part of such a function that is of interest. It follows that the boundedness of the function to be expanded, over the range of y involved, for given t, allows us to restrict consideration to functions with β real (Fourier series or integral in y). The real and imaginary parts of α yield an exponential growth or decay in time and a time dependence of the phase of the sinusoid in y, respectively. Neither of these can be excluded on a priori grounds, so α will in general be complex.

$$\frac{1}{\Delta t} e^{\alpha \Delta t} = \frac{1}{\Delta t} + \frac{pq}{(\Delta y)^2}\left[e^{i\beta \Delta y} - 2 + e^{-i\beta \Delta y}\right]$$

or

$$e^{\alpha \Delta t} = 1 + 2\frac{pq\Delta t}{(\Delta y)^2}\left[\cos(\beta \Delta y) - 1\right].$$

(As noted above, we are treating p and q as constants.)

The condition for stability (condition that all disturbances get smaller as t increases) is clearly that the real part of α should be negative for all real β, or that the quantity $e^{\alpha \Delta t}$ (which is seen to be real from the above equation) should lie between -1 and +1. From the above equation it is seen that $e^{\alpha \Delta t}$ cannot exceed +1, and the requirement that it be greater than -1 for all real β leads to the condition

(3) $2\,p\,q\,\frac{\Delta t}{(\Delta y)^2} < 1$ for stability, because the square bracket in the above equation ranges from 0 to -2 as β is varied.

Inequality (3) places severe restrictions on the choice of a mesh for numerical calculation. It is linear in Δt and quadratic in Δy. Therefore, if Δy is chosen very small in the interest of accuracy, Δt must be chosen very very small in the interest of stability. It can happen that a prohibitively large number of steps Δt would be required to complete the calculation by equation (2) over the desired domain of values of t.

III. THE IMPLICIT DIFFERENCE SYSTEM. One of us has shown[3] that the above difficulty disappears if in place of (2) we write

$$(4)\quad \frac{1}{\Delta t} F_l^{n+1} = \frac{1}{\Delta t} F_l^n + \frac{p_l^n}{2}\left[\frac{q^n_{l+\frac{1}{2}}\left(F^{n+1}_{l+1} - F^{n+1}_l\right) - q^n_{l-\frac{1}{2}}\left(F^{n+1}_l - F^{n+1}_{l-1}\right)}{(\Delta y)^2} + \frac{q^n_{l+\frac{1}{2}}\left(F^n_{l+1} - F^n_l\right) - q^n_{l-\frac{1}{2}}\left(F^n_l - F^n_{l-1}\right)}{(\Delta y)^2}\right] + G_l^n$$

(3) vonNeumann, lectures at Los Alamos, February 1947.

This set of equations is in fact unconditionally stable: that is, irregularities always decrease with increasing time t, for any choices of Δt and Δy. In this case substitution of $e^{i\beta y}\, e^{\alpha t}$ into (4) leads to

$$e^{\alpha \Delta t} - 1 = 2 \frac{pq\Delta t}{(\Delta y)^2} \left[\cos(\beta \Delta y) - 1\right] \frac{e^{\alpha \Delta t} + 1}{2}$$

or

$$\tanh \frac{\alpha \Delta t}{2} = \frac{pq\Delta t}{(\Delta y)^2} \left[\cos(\beta \Delta y) - 1\right], \text{ as the relation between } \alpha \text{ and } \beta.$$

The left hand member of this equation is negative real, and its inverse hyperbolic tangent is, therefore negative real plus an integral multiple of πi, so that the real part of α is always negative. The price one pays for this is that if we regard the F_ℓ^{n+1} ($\ell = 0, 1, 2, \cdots\cdots$) as the unknowns, system (4) is a large number of simultaneous equations, whereas each equation of the system (2) gives one of the unknowns explicitly. It may be noted in passing that (4) is a somewhat better approximation to (1) than is (2). Indeed, if we had written p_ℓ^{n+1}, $q_{\ell+\frac{1}{2}}^{n+1}$, $q_{\ell-\frac{1}{2}}^{n+1}$ instead of p_ℓ^n, $q_{\ell+\frac{1}{2}}^n$, $q_{\ell-\frac{1}{2}}^n$ in the first term of the square bracket and had written $G_\ell^{n+\frac{1}{2}}$ instead of G_ℓ^n, (4) would have been correct to second order in Δt. But if this had been done, the system would have been still more implicit, (and non-linear) because the unknowns, F_ℓ^{n+1} would have occurred in the quantities p_ℓ^{n+1} etc. Our concern here is with stability rather than with accuracy.

(4) is of interest primarily when Δy is smaller than the limit set by (3) for a given Δt. We therefore first consider (formal) methods of solving (4) in the limit $\Delta y \longrightarrow 0$. That is, we retain the differential character of the original equation (1) with respect to the variable y, and write

$$(5)\quad \frac{1}{\Delta t} F(y, t+\Delta t) = \frac{1}{\Delta t} F(y,t) + \frac{p}{2} \frac{\partial}{\partial y} q \frac{\partial}{\partial y} \left[F(y,t) + F(y, t+\Delta t)\right] + G$$

where it is understood that the variables entering implicitly through p,q,G are taken to be y, t, F(y,t). For a given value of t, (5) is essentially an <u>ordinary</u> differential equation, with $F(y, t+\Delta t)$ and y the dependent and independent variables, and with p,q,G known functions of y. We therefore call

(6) $\frac{2}{\Delta t} = \lambda =$ constant

(7) $\frac{2}{\Delta t} F(y,t) + 2G + p \frac{\partial}{\partial y} \left(q \frac{\partial F(y,t)}{\partial y} \right) = \phi = \phi(y)$

(8) $F(y, t + \Delta t) = f \equiv f(y)$

and write

(9) $\lambda f = p \frac{d}{dy} \left(q \frac{df}{dy} \right) + \phi$

IV. THE SOLUTION OF EQUATION (9). The general solution has two "constants of integration" to be fixed by the boundary conditions. For many physical problems the boundary conditions are imposed at two different points, y_1 and y_2, so that a direct stepwise numerical integration of (9) is not possible, unless a trial-and-error procedure be adopted. But such a procedure is very difficult in the present case (i.e. with $pq > 0$ and λ, ϕ large) because a solution which departs only slightly from the desired solution at one value of y departs therefrom in general more and more as the integration proceeds. The departure from the desired solution is roughly exponential in character as $y \rightarrow$ either $\pm \infty$ and grows at a rate which is greater, the smaller Δt. It is preferable to solve (9) by means of a Greene's function that can be constructed from particular solutions of the corresponding homogeneous equation (Hilbert's "paramatrix") and which causes the boundary conditions to be satisfied automatically.

It is convenient to transform (9) to the canonical form of the Sturm-Liouville theory. Introduce the new dependent and independent variables g and χ, and known functions ψ, σ as follows:

$$\chi = \int \frac{dy}{\sqrt{pq}} , \qquad \rho = \left(\frac{q}{p} \right)^{\frac{1}{4}} ,$$

$$g = \rho f , \qquad \psi = \rho \phi ,$$

$$\sigma = \frac{1}{\rho} \frac{d^2}{d\chi^2} \rho .$$

From these definitions there follows the identity

$$p\frac{d}{dy}\left(q\frac{d\Phi}{dy}\right)=\frac{1}{\rho}\left(\frac{d^2}{d\chi^2}-\sigma\right)(\rho\Phi)$$

for any function $\Phi(y)$. Then (9) becomes

$$(10)\qquad \lambda g=\left(\frac{d^2}{d\chi^2}-\sigma\right)g+\psi,$$

where

$$\psi=\left(\frac{d^2}{d\chi^2}+\lambda-\sigma\right)\left(\rho F(y,t)\right)+2\rho G$$

in which $F(y,t)$ is to be regarded as a function of χ through the relation $\chi=\int\frac{dy}{\sqrt{pq}}$.

Let the boundary condition be $g(\chi_1)=g_1$, $g(\chi_2)=g_2$.

Let $g_o(\chi)$ be a solution of the corresponding homogeneous equation, vanishing at $\chi=\chi_1$. That is, $g_o(\chi)$ satisfies

$$(11)\qquad \frac{d^2}{d\chi^2}g_o=(\lambda+\sigma)g_o,\quad g_o(\chi_1)=0.$$

Define $g_{oo}(\chi)$ by

$$(12)\qquad g_{oo}(\chi)=g_o(\chi)\int_{\chi}^{\chi_2}\frac{dz}{\left[g_o(z)\right]^2}.$$

By differentiating (12) twice and using (11), we see that $g_{oo}(\chi)$ is also a solution of the homogeneous equation. That is,

$$\frac{d^2}{d\chi^2}g_{oo}=\frac{d}{d\chi}\left[\frac{dg_o}{d\chi}\int_{\chi}^{\chi_2}\frac{dz}{\left[g_o(z)\right]^2}-\frac{1}{g_o}\right]$$

$$=\frac{d^2g_o}{d\chi^2}\int_{\chi}^{\chi_2}\frac{dz}{\left[g_o(z)\right]^2}=(\lambda+\sigma)\,g_o\int_{\chi}^{\chi_2}\frac{dz}{\left[g_o(z)\right]^2},$$

or

$$(13)\qquad \frac{d^2}{d\chi^2}g_{oo}=(\lambda+\sigma)\,g_{oo},\quad g_{oo}(\chi_2)=0$$

and furthermore

(14) $g_o(\chi)\frac{d}{d\chi}g_{oo}(\chi) - g_{oo}(\chi)\frac{d}{d\chi}g_o(\chi) = -1.$

Now define $g(\chi)$ by

(15) $$g(\chi) = g_{oo}(\chi)\left[\int_{\chi_1}^{\chi} g_o(z)\psi(z)dz + \alpha\right] + g_o(\chi)\left[\int_{\chi}^{\chi_2} g_{oo}(z)\psi(z)dz + \beta\right]$$

where α and β are two constants.

By differentiating (15) twice and using (11), (13), (14) we see that

$$\frac{d^2}{d\chi^2}g = (\lambda+\sigma)g - \psi,$$

or, in other words, that (15) is the general solution of (10). That is;

$$\frac{dg(\chi)}{d\chi} = \frac{dg_{oo}(\chi)}{d\chi}\left[\int_{\chi_1}^{\chi} g_o(z)\psi(z)dz + \alpha\right] + g_{oo}(\chi)\, g_o(\chi)\psi(\chi)$$
$$+ \frac{dg_o(\chi)}{d\chi}\left[\int_{\chi}^{\chi_2} g_{oo}(z)\psi(z)dz + \beta\right] - g_o(\chi)\, g_{oo}(\chi)\psi(\chi)$$

$$\frac{d^2g(\chi)}{d\chi^2} = \frac{d^2g_{oo}(\chi)}{d\chi^2}\left[\int_{\chi_1}^{\chi} g_o(z)\psi(z)dz + \alpha\right] + \frac{dg_{oo}(\chi)}{d\chi}\, g_o(\chi)\psi(\chi)$$
$$+ \frac{d^2g_o(\chi)}{d\chi^2}\left[\int_{\chi}^{\chi_2} g_{oo}(z)\psi(z)dz + \beta\right] - \frac{dg_o(\chi)}{d\chi}\, g_{oo}(\chi)\psi(\chi)$$
$$= (\lambda+\sigma)\, g_{oo}(\chi)\left[\int_{\chi_1}^{\chi} g_o(z)\psi(z)dz + \alpha\right]$$
$$+ (\lambda+\sigma)\, g_o(\chi)\left[\int_{\chi}^{\chi_2} g_{oo}(z)\psi(z)dz + \beta\right] - \psi(z)$$

by (11), (13), (14). The stated result then follows from definition (15).

$g_o(\chi)$ vanishes with positive slope at $\chi = \chi_1$ and increases roughly exponentially as χ increases to χ_2. Conversely, g_{oo} vanishes with negative slope at $\chi = \chi_2$ and increases roughly exponentially as χ decreases to χ_1. (See also second paragraph below.) For numerical application of this solution it is, therefore, convenient to deal with quantities defined as follows:

(16a,b) $k_o(\chi) = \dfrac{g_o(\chi)}{\frac{d}{d\chi} g_o(\chi)}$, $\qquad k_{oo}(\chi) = -\dfrac{g_{oo}(\chi)}{\frac{d}{d\chi} g_{oo}(\chi)}$;

From (11) and (13) these quantities are seen to satisfy:

(17a,b) $\frac{d}{d\chi} k_o = 1 - k_o^2 (\lambda + \sigma)$, $\qquad -\frac{d}{d\chi} k_{oo} = 1 - k_{oo}^2 (\lambda + \sigma)$,

(18a,b) $k_o(\chi_1) = 0$, $\qquad k_{oo}(\chi_2) = 0$.

Furthermore, the two terms on the right hand side of (15) will be denoted by $A(\chi)$ and $B(\chi)$ respectively. These quantities are seen to satisfy, and be fixed by the relations

(19a) $$\frac{d}{d\chi} A(\chi) = -\frac{A(\chi)}{k_{oo}(\chi)} + \frac{k_o(\chi)\, k_{oo}(\chi)}{k_o(\chi) + k_{oo}(\chi)} \psi(\chi),$$

(19b) $$-\frac{d}{d\chi} B(\chi) = -\frac{B(\chi)}{k_o(\chi)} + \frac{k_o(\chi)\, k_{oo}(\chi)}{k_o(\chi) + k_{oo}(\chi)} \psi(\chi),$$

and

(20a,b) $A(\chi_1) = g_1$, $\qquad B(\chi_2) = g_2$.

That is,

$$\frac{dA(\chi)}{d\chi} = \frac{dg_{oo}(\chi)}{d\chi}\left[\int_{\chi_1}^{\chi} g_o(z)\psi(z)\, dz + \alpha\right] + g_{oo}(\chi)\, g_o(\chi)\psi(\chi)$$

$$= -\frac{A(\chi)}{k_{oo}(\chi)} + g_{oo}(\chi)\, g_o(\chi)\psi(\chi)$$

but $$\frac{k_o\, k_{oo}}{k_o + k_{oo}} = \frac{g_{oo}\, g_o}{g_o \frac{dg_{oo}}{d\chi} - g_{oo} \frac{dg_o}{d\chi}} = g_{oo} g_o \text{ by (14)},$$

and from this (19a) follows. (19b) is similarly obtained.

The procedure for numerical calculation consists of the following steps: integrate (17a) from χ_1 to χ_2 starting with (18a) and integrate (17b) from χ_2 to χ_1 starting with (18b); then integrate (19a) from χ_1 to χ_2 and (19b) from χ_2 to χ_1 starting with (20a) and (20b) respectively; then the desired function is given by

(21) $g(\chi) = A(\chi) + B(\chi)$.

Note that in a routine involving punch cards, the integrations of (17b) and (19b) can be combined in a single pass through the card deck after the integration of (17a) has been done.

The functions k_o and k_{oo} have several advantages over g_o and g_{oo} for numerical work. If $\lambda^{\frac{1}{2}}(\chi_2-\chi_1)>>1$ (as is usually the case), the sizes of g_o and g_{oo} vary by many powers of 10 (because of their aforementioned roughly exponential character) whereas k_o and k_{oo} stay nicely in range. Furthermore, g_o and g_{oo} generally change by sizable fractions of themselves in a single step of the integration in χ, requiring the use of high order integration formulas, whereas k_o and k_{oo} are usually nearly constant over many steps of the integration. Lastly, k_o and k_{oo} can be obtained by integrating first order differential equations (17 a,b). The second of these advantages is somewhat illusory, as we will have to develop elaborate integration formulas for the k_o, k_{oo} also.

V. DIFFERENCE EQUATIONS, AGAIN. If equations (17a,b) and (19a,b) are rewritten as difference equations, we will have a system essentially equivalent to (4), although the nature of the approximation may have changed slightly by virtue of our detour through differential equation theory. The advantage gained by the operations of Section IV is, of course, that our new set of difference equations can be solved directly, whereas the set (4) cannot be, as it stands, except by inverting a matrix of order equal to the number of mesh points with given n.

Corresponding to the fixed interval size Δy in y, there will be a variable interval size

$\Delta\chi$ in χ, given by

$$(22)\quad \Delta\chi = \Delta y\,(pq)^{-\frac{1}{2}}$$

so that condition (3) for the validity of the explicit method is

$$(23)\quad (\Delta\chi)^2 > 2\Delta t \quad \text{or} \quad \sqrt{\lambda}\,\Delta\chi > 2$$

The implicit method, on the other hand, is valid, no matter what the relative sizes of $(\Delta\chi)^2$ and $2\Delta t$ may be. But when (23) holds (in fact, under all conditions except $(\Delta\chi)^2 << 2\Delta t$), one must use care in writing difference equations to approximate (17a,b) and (19 a,b). To illustrate, consider the special case of equation (17a) in

which $(\lambda+\sigma)$ is a constant and consider a solution lying close to $(\lambda+\sigma)^{-\frac{1}{2}}$ so we may write $k_0(x) = (\lambda+\sigma)^{-\frac{1}{2}} + \delta k_0(x)$. If we had made (17a) into a difference equation by writing

$$(24)\quad k_0(x_{\ell+1}) = k_0(x_\ell) + \left[1 - (\lambda+\sigma)\left\{k_0(x_\ell)\right\}^2\right](x_{\ell+1}-x_\ell),$$

then δk_0 would satisfy

$$(25)\quad \delta k_0(x_{\ell+1}) = \delta k_0(x_\ell)\left[1 - 2\sqrt{\lambda+\sigma}\ (x_{\ell+1}-x_\ell)\right]$$

instead of the correct relation

$$(26)\quad \delta k_0(x_{\ell+1}) = \delta k_0(x_\ell)\exp\left[-2\sqrt{\lambda+\sigma}\ (x_{\ell+1}-x_\ell)\right]$$

derivable from the differential equation. Clearly (25) agrees with (26) if $\sqrt{\lambda+\sigma}\ (x_{\ell+1}-x_\ell) << 1$ but not otherwise. Indeed, if $\sqrt{\lambda+\sigma}\ (x_{\ell+1}-x_\ell) > 1$, the $\delta k_0(x)$ computed from (25) increases in magnitude exponentially as x increases, instead of decreasing exponentially as it should. Thus the implicit method acquires a sort of instability under just those conditions where the explicit method is stable.

We avoid the instability (and also the inaccuracy) that would result from use of (25) as follows: to obtain a formula (alternative to (25)) for calculating $k_0(x_{\ell+1})$ from $k_0(x_\ell)$, we solve (17a) analytically in each interval $(x_\ell, x_{\ell+1})$ under the assumption that $\lambda+\sigma$ is constant in this interval. The general solution is

$$(27)\quad \sqrt{\lambda+\sigma}\ k_0(x) = \frac{e^{2\sqrt{\lambda+\sigma}\,(x-x_\ell)} - A_0}{e^{2\sqrt{\lambda+\sigma}\,(x-x_\ell)} + A_0},$$ where A_0 is a constant.

We give σ its value $\sigma_{\ell+\frac{1}{2}}$ at the midpoint of the interval; we determine A_0 in terms of the known $k_0(x_\ell)$ by setting $x = x_\ell$; and then we set $x = x_{\ell+1}$ in (27). The result is

$$(28)\quad \sqrt{\lambda+\sigma_{\ell+\frac{1}{2}}}\ k_0(x_{\ell+1}) = \frac{\left[1+\sqrt{\lambda+\sigma_{\ell+\frac{1}{2}}}\ k_0(x_\ell)\right] e^{2\omega} - \left[1-\sqrt{\lambda+\sigma_{\ell+\frac{1}{2}}}\ k_0(x_\ell)\right]}{\left[1+\sqrt{\lambda+\sigma_{\ell+\frac{1}{2}}}\ k_0(x_\ell)\right] e^{2\omega} + \left[1-\sqrt{\lambda+\sigma_{\ell+\frac{1}{2}}}\ k_0(x_\ell)\right]},$$

$$= \frac{\tanh\omega + \sqrt{\lambda+\sigma_{\ell+\frac{1}{2}}}\ k_0(x_\ell)}{1 + (\tanh\omega)\sqrt{\lambda+\sigma_{\ell+\frac{1}{2}}}\ k_0(x_\ell)}$$

where

$$(29) \quad \omega = \sqrt{\lambda + \sigma_{\ell+\frac{1}{2}}}\,(\chi_{\ell+1} - \chi_\ell).$$

The formula for $k_{oo}(\chi)$ is the same except for interchange of $\chi_{\ell+1}$ and χ_ℓ in (28) (but not in (29)).

Equation (19a) for $A(\chi)$ may be similarly treated by assuming $k_o(\chi)$ and $k_{oo}(\chi)$ constant in an interval $(\chi_{\ell-1}, \chi_\ell)$. It is advantageous not to assume that $\psi(\chi)$ is constant, for reasons that will appear later. The solution which reduces to the correct value $A_{\ell-1}$ at $\chi = \chi_{\ell-1}$ is

$$(30) \quad A(\chi) = A_{\ell-1}\, e^{-(\chi - \chi_{\ell-1})/k_{oo}} + \frac{k_o k_{oo}}{k_o + k_{oo}}\, e^{-(\chi - \chi_{\ell-1})/k_{oo}} \cdot \int_{\chi_{\ell-1}}^{\chi} e^{(\xi - \chi_{\ell-1})/k_{oo}}\, \psi(\xi)\, d\xi ,$$

or

$$(31) \quad A_\ell = A_{\ell-1}\, e^{-(\chi_\ell - \chi_{\ell-1})/k_{oo}} + \frac{k_o k_{oo}}{k_o + k_{oo}} \left[\int_{-\infty}^{\chi_\ell} e^{(\xi - \chi_\ell)/k_{oo}}\, \psi(\xi)\, d\xi - e^{-(\chi_\ell - \chi_{\ell-1})/k_{oo}} \int_{-\infty}^{\chi_{\ell-1}} e^{(\xi - \chi_{\ell-1})/k_{oo}}\, \psi(\xi)\, d\xi \right]$$

Calling $z = \frac{\chi - \xi}{k_{oo}}$, we have generally

$$\int_{-\infty}^{\chi} e^{(\xi - \chi)/k_{oo}}\, \psi(\xi)\, d\xi = k_{oo} \int_0^{\infty} e^{-z}\, \psi(\chi - k_{oo} z)\, dz$$

$$= k_{oo} \int_0^{\infty} e^{-z} \left\{ \psi(\chi) - \frac{k_{oo} z}{1!}\, \psi'(\chi) + \frac{k_{oo}^2 z^2}{2!}\, \psi''(\chi) - \cdots \right\} dz$$

$$= k_{oo}\, \chi_{oo}(\chi)$$

where primes denote differentiation with respect to χ, and

$$(32) \quad \chi_{oo}(\chi) = \psi(\chi) - k_{oo}\, \psi'(\chi) + k_{oo}^2\, \psi''(\chi) - k_{oo}^3\, \psi'''(\chi) + \cdots\cdots .$$

Then, calling

$$(33) \qquad \omega_{oo} = \frac{\chi_\ell - \chi_{\ell-1}}{k_{oo}} \ ,$$

we have, in place of (31),

$$(34) \quad A_\ell = A_{\ell-1} e^{-\omega_{oo}} + \frac{k_o k_{oo}^2}{k_o + k_{oo}} \left[\chi_{oo}(\chi_\ell) - e^{-\omega_{oo}} \chi_{oo}(\chi_{\ell-1}) \right]$$

The integration formula for $B(\chi)$ is quite similar. Calling

$$(35) \quad \chi_o(\chi) = \psi(\chi) + k_o \psi'(\chi) + k_o^2 \psi''(\chi) + k_o^3 \psi'''(\chi) + \cdots\cdots \ ,$$

and

$$(36) \quad \omega_o = \frac{\chi_{\ell+1} - \chi_\ell}{k_o} \ ,$$

the formula is

$$(37) \quad B_\ell = B_{\ell+1} e^{-\omega_o} + \frac{k_o^2 k_{oo}}{k_o + k_{oo}} \left[\chi_o(\chi_\ell) - e^{-\omega_o} \chi_o(\chi_{\ell+1}) \right]$$

For practical calculation, expressions (32) and (35) must of course be truncated. In order to see how to do this in a reasonable way, we regard the entire development so far as amounting to an expansion of the solution of the original equation (1) in powers of the small quantity Δt; or in inverse powers of the large quantity λ. For example, since the error in (5) as written is at most of first order in Δt, we may regard (9) as being correct as written, and add $O(\Delta t)$ to the first member of (7). Therefore we may regard (10) as being correct as written, and write for ψ:

$$(38) \quad \psi = \left(\frac{d^2}{d\chi^2} + \lambda - \sigma \right) \left(\rho F(y,t) \right) + 2\rho G + O\left(\frac{1}{\lambda}\right) .$$

The order of magnitude, in λ, of k_o can be found as follows: (17a) and (18a) yield formally, for given χ:

$$\int_0^{k_o(\chi)} \frac{dk}{1-(\lambda+\sigma)k^2} = \chi - \chi_1 \ .$$

In this integral, the symbol σ stands for a function of k and λ obtained by substituting for χ in the function $\sigma(\chi)$ the inverse $\chi(k)$ of the function $k_o(\chi)$.

But we shall assume that $\sigma(\chi)$ is bounded in the interval $\chi_1 \leq \chi \leq \chi_2$ so that in any case $\sigma << \lambda$ asymptotically, or

$$\chi - \chi_1 \sim \int_0^{k_0(\chi)} \frac{dk}{1-\lambda k^2} = \frac{1}{\sqrt{\lambda}} \int_0^{\sqrt{\lambda} k_0(\chi)} \frac{dp}{1-p^2}$$

or $\sqrt{\lambda}\, k_0 \sim \tanh \sqrt{\lambda}\,(\chi - \chi_1)$ as $\lambda \to \infty$.

so

(39) $k_0(\chi) = \mathcal{O}(\lambda^{-\frac{1}{2}})$ for fixed χ.

By means of (38) and (39) we now write out explicitly the expression (32) for $\chi_{oo}(\chi)$, retaining only terms down to order $\lambda^{-\frac{1}{2}}$. The result is:

$$\begin{aligned}(40)\quad \chi_{oo}(\chi) = {} & \lambda \rho F(y,t) \\ & - k_{oo} \lambda \frac{d}{d\chi} (\rho F(y,t)) \\ & + (1 + k_{oo}^2 \lambda) \frac{d^2}{d\chi^2} (\rho F(y,t)) - \sigma \rho F(y,t) + 2\rho G \\ & - k_{oo} \frac{d}{d\chi} \left[\left(\frac{d^2}{d\chi^2} - \sigma \right) (\rho F(y,t)) + 2\rho G \right] \\ & + O\left(\frac{1}{\lambda}\right).\end{aligned}$$

This equation has been so written that the first four lines contain terms in $\lambda, \lambda^{\frac{1}{2}}, 1, \lambda^{-\frac{1}{2}}$, respectively.

The corresponding expression for $\chi_o(\chi)$ is the same except for replacement of k_{oo} by $-k_o$.

Equations (28), (29), (34), (37), (40) are the final formulas. It is understood that in (40) the derivatives are to be replaced in the usual way by difference ratios, e.g.,

$$\frac{\rho_{l+1} F^n_{l+1} - \rho_{l-1} F^n_{l-1}}{\chi_{l+1} - \chi_{l-1}} \to \left[\frac{d}{d\chi} (\rho F(y,t)) \right]_{\chi = \chi_l}.$$

VI. ASYMPTOTIC EQUIVAIENCE TO THE EXPLICIT METHOD. The explicit method (see Section II, especially equations (2), (3)) is stable for $\lambda > 4/(\Delta\chi)^2$, and we shall now show that the two methods are in approximate agreement for sufficiently large values of λ. The reader may tend to regard it as self-evident that this should be true, because both methods purport to solve the original equation (1) approximately. But because actual convergence proofs are lacking for both methods, it is worthwhile to show the equivalence, especially since the two methods appear to do quite different things. The explicit method deals with local conditions: it gives F_ℓ^{n+1} in terms of the values $F_{\ell+1}^n$, F_ℓ^n, $F_{\ell-1}^n$ of F at neighboring mesh points, whereas the implicit method makes F_ℓ^{n+1} depend on F at all the mesh points of cycle n, and also on distant boundary conditions.

Before demonstrating the equivalence, we first carry the argument leading to the estimate (39) a little farther. We seek a solution of the equation

$$(41)\quad \frac{dk_o(\chi)}{d\chi} = 1 - (\lambda + \sigma)\left[k_0(\chi)\right]^2$$

in the form

$$(42)\quad k_o = \lambda^{-\frac{1}{2}}\left[a_o + a_1\lambda^{-\frac{1}{2}} + a_2\lambda^{-1} + a_3\lambda^{-3/2} + \cdots\right],$$

where the coefficients a_o, a_1, a_2, ... are functions of χ. By substitution of (42) into (41) and equating coefficients of the various powers of λ, we find $a_o \equiv 1$, $a_1 = 0$, $a_2 = -\frac{1}{2}\sigma$, $a_3 = \frac{1}{4}\frac{d\sigma}{d\chi}$, etc. We note parenthetically that the series so obtained fails to satisfy the boundary condition that $k_0(\chi_1)$ should vanish identically in λ. Apparently one must add to (42) a function of χ and λ which vanishes, as $\lambda \to \infty$, more rapidly than any inverse power of λ. The presence of such terms was foreshadowed by the appearance of exponentials, as for example in the hyperbolic tangent immediately preceding equation (39). But in any case we can write

$$(43)\quad k_o(\chi) = \lambda^{-\frac{1}{2}} - \tfrac{1}{8}\sigma\lambda^{-3/2} + \tfrac{1}{4}\frac{d\sigma}{d\chi}\lambda^{-2} + \mathcal{O}\left(\lambda^{-5/2}\right)$$

and similarly

$$k_{oo}(\chi) = \lambda^{-\frac{1}{2}} - \tfrac{1}{2}\sigma\lambda^{-3/2} - \tfrac{1}{4}\frac{d\sigma}{d\chi}\,\lambda^{-2} + \mathcal{O}\left(\lambda^{-5/2}\right).$$

For sufficiently large λ, $\omega_{oo} = \dfrac{\chi_{\ell} - \chi_{\ell-1}}{k_{oo}} \approx \lambda^{\frac{1}{2}}(\chi_{\ell} - \chi_{\ell-1})$ is $>> 1$ and similarly $\omega_{o} >> 1$, so we may replace $e^{-\omega_{oo}}$ and $e^{-\omega_{o}}$ by zero in (34) and (37).

Then

$$g(\chi_{\ell}) = A_{\ell} + B_{\ell} = \rho F(y_{\ell}, t + \Delta t) = \frac{k_o\, k_{oo}}{k_o + k_{oo}}\left[k_{oo}\chi_{oo} + k_o\chi_o\right]$$
$$\approx \tfrac{1}{2}\left(\lambda^{-\frac{1}{2}} - \tfrac{1}{2}\sigma\lambda^{-3/2}\right)^2\left[\chi_{oo} + \chi_o\right]$$

or

$$g(\chi) \approx \frac{1}{2\lambda}\left(1 - \frac{\sigma}{\lambda}\right)\left[2\lambda\rho F(y,t) + 2\left(1 + (1 - \frac{\sigma}{\lambda})\right)\frac{d^2}{d\chi^2}\quad(\rho F(y,t))\right.$$
$$\left. - 2\sigma\rho F(y,t) + 4\rho G\right],$$

or

$$(44)\quad \rho F(y, t+\Delta t) \approx \frac{1}{\lambda}\left[\lambda\rho F(y,t) + 2\frac{d^2}{d\chi^2}(\rho F(y,t)) - 2\sigma\rho F(y,t) + 2\rho G\right].$$

This can be rewritten, using the identity preceding equation (10), and the definition $\lambda = \dfrac{2}{\Delta t}$, as

$$(45)\quad \frac{F(y,t+\Delta t)}{\Delta t} = \frac{F(y,t)}{\Delta t} + p\frac{\partial}{\partial y}\left(q\frac{\partial}{\partial y}\,F(y,t)\right) + G$$

which leads immediately to the "explicit" equation (2), as was to be shown. Equation (45) is to be contrasted with equation (5) which was our starting point.

As a final remark, it is noted that near a boundary at $\chi = \chi_1$, or $\chi = \chi_2$, we must either choose the mesh size so that $(\Delta\chi)^2 << 2\Delta t$ or insure that the boundary is in a place where errors do not matter. For if $\sqrt{\lambda}\,\Delta\chi$ is of order unity or greater, it is seen from (17 a,b) and (18 a,b) that k_o or k_{oo} will vary by a large fraction in an interval $\Delta\chi$ near the boundary, contrary to the assumption underlying the derivation of (30) et seq.

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