Finite Difference Schemes for Differential Equations

By Milton E. Rose

Introduction. Consider the boundary value problem

$$Lu(x) = f(x), \qquad a < x < b$$

$$u(a) = u(b) = 0$$

for the positive definite Sturm-Liouville operator

$$L = -\frac{d}{dx}\,p(x)\,\frac{d}{dx} + q(x) \tag{1}$$

and the related variational problem for the functional

$$Q(u) = \int_a^b (pu'^2 + qu^2)\,dx - 2\int_a^b fu\,dx \tag{2}$$

viz.,

$$\min_{u \in \Omega} Q(u)$$

where the class Ω consists of smooth functions $u(x)$ satisfying $u(a) = u(b) = 0$. Following Ritz, the solution of the variational problem may be discussed within the framework of the direct methods of the calculus of variations [1] by extending Ω to the class of continuous functions with piecewise smooth derivatives. For purposes of deriving finite difference equations for the boundary value problem it is usual to consider continuous piecewise linear functions which reduce (2) to an easily evaluated sum, the Euler equations for which yield the difference equations. Thus, if $p = 1$, this results in approximating u'' by the second difference quotient $(u_{i+1} - 2u_i + u_{i-1})/\Delta x^2$. However, for problems with singular points this simple procedure may fail [10].

In this paper we illustrate certain theoretical and computational advantages which result for difference schemes by considering a canonical class of approximating functions chosen as piecewise smooth solutions of $Lu = 0$. In this case the resulting minimizing sequences for (2) lead, via the Euler equations for $Q(u)$, to a system of difference equations $\Lambda\hat{u} = \hat{f}$ where $\Lambda = (\Lambda_{ij})$ is a symmetric, tri-diagonal matrix. We call difference equations derived in this manner *patch equations*. The solution, for a given subdivision of (a, b) by points $x_1, x_2, \cdots, x_n$, is $\hat{u} = (u(x_1), u(x_2), \cdots, u(x_n))$ where $u(x)$ is the solution of $Lu = f$. Moreover, if $K(x, y)$ is the Green's function for L on (a, b), so that $LK = \delta(x - y)$, we also have $\sum_{j=1}^n K(x_i, x_j)\Lambda_{jk} = \delta_{ik}$. Thus the structure of such difference equations parallels that of the differential equation.

The more familiar analytical approximation to (1) based upon expansions with a complete set of functions also permits a parallel development here. Corresponding

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to a given subdivision of the interval (a, b) one may introduce a basis $\{r_i(x)\}$ for which the finite difference equations express conditions determining the coefficients of $u(x) = lim_{n\to\infty} \sum_{i=1}^{n} u_i r_i(x)$.

The first part of this paper develops this formalism for Sturm-Liouville problems; its application to several examples are given in (I.2) in order to illustrate certain novel features of the resulting difference equations. In the second part we investigate selected aspects of the method for partial differential equations. A discussion of the approximate solution of the difference equations corresponding to elliptic problems by certain "alternating direction" methods, for example, is possible in a simple manner. Finally, an extension of the method to the heat equation is described; by way of illustration a somewhat novel scheme which may be suitable for calculating temperatures inside a circular plate is discussed (Example D).

I. Difference Equations for Sturm-Liouville Operators

I.1 Patch Difference Equations. For the purpose of introducing notations which will be used throughout this paper it will be convenient to review the derivation of finite difference equations appropriate to the Sturm-Liouville problem

$$\begin{aligned} Lu(x) &= f(x), \\ u(a) &= u(b) = 0 \qquad a < x < b \end{aligned} \tag{3}$$

by means of variational arguments (for simplicity we shall limit our present discussion to the case in which L, given by (1), is non-singular on (a, b)).

Consider a fixed but arbitrary subdivision of the interval (a, b) by points $a = x_0, x_1, \cdots, x_{n+1} = b$. Let $r_i^+(x)$ denote the solution of $Lu = 0$ in (x_i, x_{i+1}) for which $u(x_i) = 1$, $u(x_{i+1}) = 0$ and let $r_i^-(x)$ denote the corresponding solution in (x_{i-1}, x_i) for which $u(x_{i-1}) = 0$, $u(x_i) = 1$. The functions

$$r_i(x) = \begin{cases} r_i^+(x), & x_i \leqq x \leqq x_{i+1} \\ r_i^-(x), & x_{i-1} \leqq x \leqq x_i \\ 0, & x \notin (x_{i-1}, x_{i+1}), \end{cases}$$

$i = 1, 2, \cdots, n$, defined on the set of overlapping intervals $\{(x_{i-1}, x_{i+1})\}$ forming a patch-like covering (a, b) will be called a *patch basis* for the operator L on (a, b); Ω_n denotes the manifold spanned by the basis $\{r_i(x)\}$. Since $r_i(x_j) = \delta_{ij}$, if $u^n(x) \in \Omega_n$ then $u^n(x) = \sum_{i=1}^{n} u^n(x_i) r_i(x)$ and $u^n(x_0) = u^n(x_{n+1}) = 0$. Clearly, if $K_i(x, x)$ denotes the Green's function for L on the patch (x_{i-1}, x_{i+1}), $r_i(x) = K_i(x,x_i)/K_i(x_i, x_i)$, $i = 1, 2, \cdots, n$.

Finally, we introduce the inner product

$$(u, v) = \int_a^b u(x)v(x)\, dx$$

and extend L on Ω_n as the symbolic function

$$\begin{aligned} Lr_i(x) = p(x_{i+1})&r_i'(x_{i+1}-)\delta(x - x_{i+1}) \\ &- p(x_i)[r_i'(x_i+) - r_i'(x_i-)]\delta(x - x_i) \\ &\qquad - p(x_{i-1})r_i'(x_{i-1}+)\delta(x - x_{i-1}) \end{aligned} \tag{4}$$

where $r_i'(\xi\pm) = \dfrac{d}{dx} r_i(\xi\pm)$. Throughout this paper we shall assume this extention without separate comment. Thus, for $u^n(x) = \sum_{i=1}^n u_i^n r_i(x)$, we shall write

$$Lu^n(x) = \sum_{i=1}^n u_i^n Lr_i(x)$$

and

$$(r_j, Lu^n) = \sum_{i=1}^n u_i^n (r_j, Lr_i).$$

The formula

$$\sum_{i=1}^n p(\xi) u^{n'}(\xi) u^n(\xi) \Big|_{\xi=x_i+}^{\xi=x_i+1^-} = \sum_{i,j=1}^n u_i^n u_j^n (r_i, Lr_j) = (u^n, Lu^n)$$

results by writing $u^{n'}(x_{i+1}-) = u_{i+1}^n r'_{i+1}(x_{i+1}-) + u_i^n r_i'(x_{i+1}-)$, etc. and rearranging terms. Hence, for $u^n(x) \in \Omega_n$, the quadratic functional $Q(u^n)$ given in (2) is easily evaluated:

$$Q(u^n) = \sum_{i=0}^n \left\{ p(\xi) u^{n'}(\xi) u^n(\xi) \Big|_{\xi=x_i+}^{\xi=x_i+1^-} - 2\int_{x_i}^{x_i+1} u^n(\xi) f(\xi)\, d\xi \right\}$$
$$= (u^n, Lu^n) - 2(u^n, f);$$

this corresponds to the formula $Q(u) = (u, Lu) - 2(u, f)$ for smooth functions $u(x)$. The Euler equations for

$$\min_{u^n \in \Omega_n} Q(u^n)$$

may be expressed as

$$(Lu^n - f, \delta u^n) = 0$$

for arbitrary $\delta u^n \in \Omega_n$; equivalently

$$(5) \qquad \sum_{j=1}^n (r_i, Lr_j) u_j^n = (r_i, f), \qquad i = 1, 2, \cdots, n$$

or, more explicitly,

$$p(x_{i+1}) r_i'(x_{i+1}-) u_{i+1}^n - p(x_i)[r_i'(x_i+) - r_i'(x_i-)] \cdot u_i^n$$

$$(5') \qquad - p(x_{i-1}) r_i'(x_{i-1}+) u_{i-1}^n = \int_{x_i-1}^{x_i+1} r_i(x) f(x)\, dx,$$

$$i = 1, 2, \cdots, n$$

with $u_0^n = u_{n+1}^0 = 0$.

The system (5) (or (5′)) furnishes a system of finite difference equations appropriate for the solution of (3). To emphasize their particular form we shall call them the *patch equations* corresponding to problem (3).

The matrix $((r_i, Lr_j))$ is symmetric and tri-diagonal, the latter being apparent from (4). To show the symmetry, since $Lr_i(x) = Lr_{i-1}(x) = 0$ in (x_{i-1}, x_i), Green's formula yields

$$0 = \int_{x_{i-1}}^{x_{i+1}} \{r_i(x)Lr_{i-1}(x) - r_{i-1}(x)Lr_i(x)\}\,dx$$

$$= p(x_i)r'_{i-1}(x_i-) - p(x_{i-1})r_i'(x_{i-1}+)$$

so that, noting the relations $(r_i\,,\,Lr_{i-1}) = p(x_i)r'_{i-1}(x_i-)$ and $(r_{i-1}\,,\,Lr_i) = p(x_{i-1})r_i'(x_{i-1}+)$, we obtain $(r_i\,,\,Lr_{i-1}) = (r_{i-1}\,,\,Lr_i)$.

For smooth functions admissible to the original variational problem, $w(x) \in \Omega$, the function

$$T_nw(x) = \sum_{i=1}^{n} w(x_i)r_i(x)$$

in Ω_n interpolates to $w(x_i)$ at $x = x_i\,, i = 0, 1, \cdots, n + 1$. A simple, but important result is that the solution $u^n(x)$ of the patch equations (5) is given by $T_nu(x)$ where $u(x)$ is the solution of (3), i.e., the solution values $u(x_i)$ necessarily satisfy the patch equations (5′). For, clearly, if $u(x)$ is the solution of (3),

$$\int_{x_{i-1}}^{x_{i+1}} K_i(x, y)[Lu(x) - f(x)]\,dx = 0, \qquad i = 1, 2, \cdots, n$$

where $K_i(x, y)$ is the Green's function for L on $(x_{i-1}\,, x_{i+1})$. Thus

$$p(x_{i+1})K_i(x_{i+1}\,, y)u(x_{i+1}) - p(x_{i-1})K_i(x_{i-1}\,, y)u(x_{i-1}) + u(y)$$

$$= \int_{x_{i-1}}^{x_{i+1}} K_i(x, y)f(x)\,dx, \quad i = 1, \cdots, n.$$

These last equations furnish a system of connection formulae between the values of $u(y)$ on the patch intervals. Setting $y = x_i$ in the ith equation, placing $r_i(x) = K_i(x, x_i)/K_i(x_i\,, x_i)$ and recalling that $K_i'(x_{i}+\,, x_i) - K_i'(x_{i}-\,, x_i) = -1/p(x_i)$ we obtain (5′).

We shall illustrate the form of the patch equations in specific examples in Section I.2. For the present we merely note that the treatment of a more general boundary condition of the form $u'(b) + \beta u(b) = 0$, say, may be accomplished by requiring that the Green's function $K_n(x, y)$ (and, correspondingly, the patch function $r_n(x)$) satisfy the same condition at $x = b$. A similar modification is possible for certain singular problems. For the validity of our discussion in such cases it is only necessary to modify (4) appropriately; we shall assume this to have been accomplished without separate mention of the fact.

It will, in practice, be necessary in general to approximate the values $(r_i\,, f)$ occurring in the right hand terms of (5) by approximate values, say $(r_i\,, f_n)$, where $(r_i, f_n) \to (r_i\,, f)$ for $n \to \infty$. If $\tilde{u}^n(x) \in \Omega_n$ is the resulting approximate solution it will be useful, then, to obtain an estimate for $\max_x |\,\tilde{u}^n(x) - u(x)\,|$. To accomplish this we shall show that

$$T_nu(x) = \int_a^b K^n(x, y)f(y)\,dy$$

where $K^n(x, y)$ is a separable kernel on $\Omega_n \times \Omega_n$ which approximates the Green's function $K(x, y)$ for L on (a, b).

We recall that the patch function $r_i(x)$ is obtained by normalizing the Green's function $K_i(x, x_i)$ on the patch (x_{i-1}, x_{i+1}) and extending it by vanishing outside the interval. Denote the subinterval (x_i, x_{i+1}) by J_i, $i = 0, 1, \cdots, n$ and let $K(x, y \mid J_i)$ denote the Green's function for L on J_i extended so as to vanish wherever x or y or both lie outside J_i.

THEOREM. *Let*

$$K^n(x, y) = \sum_{i,j=1}^{n} K(x_i, x_j)r_i(x)r_j(y)$$

and

$$H^n(x, y) = \sum_{i=0}^{n} K(x, y \mid J_i).$$

Then

$$K(x, y) = K^n(x, y) + H^n(x, y)$$

and

$$\lim_{n\to\infty} K^n(x, y) = K(x, y)$$

uniformly for x, y *in* (a, b).

We sketch the proof. First note that $r_i(x)$ is a piecewise smooth solution of $Lu(x) = 0$ with $r_i(x_j) = \delta_{ij}$. Suppose $y \in J_j$, $x \notin J_j$. Then, for fixed y, $K(x, y) - K^n(x, y)$ is a regular solution of $Lu(x) = 0$ in each interval $J_i (i \neq j)$ which vanishes at the end points. Hence $K(x, y) = K^n(x, y)$ for $x \notin J_j$. When $x \in J_j$, $K^n(x, y)$ is a regular solution of $Lu(x) = 0$ with boundary values equal to $K(x_j, y)$ and $K(x_{j+1}, y)$, while $H^n(x, y)$ is a solution of $Lu(x) = \delta(x - y)$ which vanishes at x_j and x_{j+1}. Thus $K(x, y) = K^n(x, y) + H^n(x, y)$.

Now note that $H^n(x, y)$ contains at most one non-zero term so that, since the jump in the derivative of $K(x, y \mid J_i)$ is normalized at $x = y$,

$$| H^n(x, y) | \leqq \max_{x,y} | K(x, y \mid J_i) | \leqq c| J_i |.$$

Thus the theorem easily follows.

The solution of (3) may be represented through the Green's function as

$$u(x) = \int_a^b K(x, y)f(y)\, dy$$

and, as we have indicated, the solution of the patch equations (5) may be represented, uniquely in Ω_n, as

$$T_n u(x) = \sum_{i=1}^{n} u(x_i)r_i(x).$$

Since $H^n(x_i, y) = 0$, clearly, then,

$$T_n u(x) = \sum_{i=1}^{n} \left(\int_a^b K(x_i, y)f(y)\right) r_i(x) = \int_a^b \left(\sum_{i=i}^{n} K^n(x_i, y)r_i(x)\right) f(y)\, dy$$

or

$$T_n u(x) = \int_a^b K^n(x, y) f(y)\, dy. \tag{6}$$

Thus, if

$$\tilde{u}^n(x) = \int_a^b K^n(x, y) f_n(y)\, dy,$$

we obtain the desired truncation estimate

$$\max_x | \tilde{u}^n(x) - u(x) | \leqq \max_x \left| \int_a^b K^n(x, y)[f_n(y) - f(y)]\, dy \right| + \max_x \left| \int_a^b H^n(x, y) f(y)\, dy \right|.$$

If we note that (6) is equivalent to

$$u(x_i) = \sum_{j=1}^n K(x_i, x_j)(r_j, f)$$

we may summarize our results as follows:

To solve $Lu = f$ on (a, b), $u(a) = u(b) = 0$, for values of the solution $u(x)$ at an arbitrary set of points $x_1, x_2, \cdots, x_n$ of subdivision of (a, b), first construct the patch basis $\{r_i(x)\}$; then the function $u^n(x) \in \Omega_n$ which interpolates to $u(x)$ at $x_1, x_2, \cdots, x_n$ solves the variational problem

$$\min_{\phi^n \in \Omega_n} Q(\phi^n),$$

i.e., the solution $u^n(x)$ satisfies the Euler conditions

$$(Lu^n - f, \phi^n) = 0$$

for arbitrary $\phi^n(x) \in \Omega_n$. The solution of the system of patch equations

$$\sum_{i=1}^n (r_j, Lr_i) u_i^n = (f, r_j), \qquad j = 1, 2, \cdots, n$$

resulting from the preceding orthogonality conditions is given by $u_i^n = u(x_i)$ and

$$u(x_i) = \sum_{j=1}^n K(x_i, x_j)(r_j, f), \qquad i = 1, 2, \cdots, n.$$

Thus, also,

$$\sum_{j=1}^n (r_i, Lr_j) K(x_j, x_k) = \delta_{ik}.$$

For the more general problem $Lu(x) + s(x)u(x) = f(x)$ the interpolation $T_n u(x)$ need no longer satisfy the corresponding patch equations $(r_i, Lu^n + su^n - f) = 0$, $i = 1, 2, \cdots, n$. Nevertheless the solutions $u^n(x)$, considered either as minimizing sequences for the variational problem or as solutions of the integral equation

$$u^n(x) + \int_a^b K^n(x, y) s(y) u^n(y)\, dy = \int_a^b K^n(x, y) f(y)\, dy$$

may be shown to converge to $u(x)$ (cf. Section I.2, Example C.).

In practice the construction of a patch basis for L itself may be difficult to achieve. A similar difficulty often arises also in attempting an approximation by an expansion using a basis formed by the eigenfunctions of L; in this case one may attempt to write $L = M + N$ where an eigenfunction basis for M is known and where N may be treated as a perturbation. An analogous procedure applies also in the treatment of difference equations; in fact, by choosing a sufficiently small mesh interval, the operator $-\frac{d^2}{dx^2}$ may usually be chosen to furnish a patch basis.

I.2 Examples of Patch Difference Equations. The following examples may serve to illustrate the discussion of the previous section.

Example A.

$$Lu(x) \equiv -\frac{d^2u(x)}{dx^2} = f(x), \qquad 0 < x < 1,$$

with $u(0) = u_0$, $u'(1) + u(1) = 0$.

Assuming a uniform subdivision of $(0, 1)$ by points $x_k = kh$, $k = 0, 1, \cdots, n + 1$, we have for $i = 1, 2, \cdots, n - 1$,

$$r_i(x) = \begin{cases} (x - x_{i+1})/h, & x_{i+1} \geqq x \geqq x_i \\ (x - x_{i-1})/h, & x_i \geqq x \geqq x_{i-1} \end{cases}$$

and, for $i = n$,

$$r_n(x) = \begin{cases} (x - 2)/(x_n - 2), & 1 \geqq x \geqq x_n \\ (x - x_{n-1})/h, & x_n \geqq x \geqq x_{n-1} \end{cases}$$

while $r_i(x) = 0$ for $x \notin (x_{i-1}, x_{i+1})$, $i = 1, 2, \cdots, n$. From (4),

$$Lr_i(x) = -\frac{1}{h}[\delta(x - x_{i+1}) + \delta(x - x_{i-1})] + \frac{2}{h}\delta(x - x_i), \qquad i \neq n$$

and

$$Lr_n(x) = -\frac{1}{h}\delta(x - x_{n-1}) + \frac{(2h + 1)}{h(h + 1)}\delta(x - x_n),$$

so that the conditions

$$(r_i, Lu^n - f) = 0, \qquad i = 1, 2, \cdots, n$$

lead to equations

$$\mathrm{A}_1: \qquad -\frac{1}{h}(u_{i+1}^n + u_{i-1}^n) + \frac{2}{h}u_i^n = (r_i, f), \qquad i \neq n$$

and

$$\mathrm{A}_2: \qquad -\frac{1}{h}u_{n-1}^n + \frac{(2h + 1)}{h(h + 1)}u_n^n = (r_n, f),$$

with $u_0^n = u_0$.

In the present case, equation A_2 may be obtained by applying A_1 when $i = n$ and using the first order difference approximation $(u_{n+1}^n - u_n^n)/h + u_{n+1}^n = 0$ to the boundary condition $u'(1) + u(1) = 0$. On the basis of our earlier remarks we may conclude that the introduction of a higher order difference approximation to this boundary condition (sometimes suggested) cannot improve the approximation.

Example B. To illustrate the treatment of an operator with a singular point consider

$$L_u(x) \equiv -\frac{d}{dx}\, x\, \frac{d}{dx}\, u(x) + \frac{1}{x}\, u(x) = 1, \qquad 0 < x < 1$$

with $u(0)$ finite and $u(1) = 0$. The solution of this problem is $u(x) = -\frac{1}{2}\, x \log x$, the origin being a singular point of the differential equation.

With respect to a given subdivision of the interval $(0, 1)$ the patch functions are

$$r_i(x) = \begin{cases} x_i(x^2 - x_{i-1}^2)/x\Delta_i\,, & x_{i-1} \leqq x \leqq x_i \\ x_i(x_{i+1}^2 - x^2)/x\Delta_{i+1}\,, & x_i \leqq x \leqq x_{i+1} \\ 0, & x \geqq x_{i+1}\,, x \leqq x_i \end{cases}$$

where $\Delta_i = x_i^2 - x_{i-1}^2$. The patch equations (5) assume the form

$$-2x_i\left[\frac{x_{i+1}u_{i+1}^n}{\Delta_{i+1}} + \frac{x_{i-1}u_{i-1}^n}{\Delta_i}\right] + 2x_i^2\left[\frac{1}{\Delta_i} + \frac{1}{\Delta_{i+1}}\right]u_i^n = (r_i\,,\, 1),$$
$$i = 1, 2, \cdots, n.$$

Noting that the coefficient of u_0^n vanishes we see that the condition $u_{n+1}^n = 0$ insures the unique solution of this system.

Example C. Consider

$$Lu(x) \equiv -u''(x) + \rho^2(x)u(x) = g(x), \qquad 0 < x < \infty$$

with

$$u(0) = 0, \qquad u(\infty) = 0.$$

A familiar treatment of this problem is to consider a succession of approximations on finite intervals $(0, R)$ as $R \to \infty$. On each such interval a patch basis with respect to $-d^2/dx^2$ may be used to construct a system of integral equations expressing connection formula for values of the solution between patch intervals as described at the end of the last section.

A more novel treatment is the following: Let $0 = x_0\,, x_1\,, \cdots, x_{n+1} = \infty$ and, on the interval $(x_{i-1}\,, x_{i+1})$, let

$$L_i u(x) = -u''(x) + \rho^2(x_i)u(x)$$

and let $r_i(x)$ denote the patch function obtained by normalizing the Green's function for L_i on $(x_{i-1}\,, x_{i+1})$. Then, with $\rho_i = \rho(x_i)$,

$$r_i(x) = \begin{cases} \sinh \rho_i(x - x_{i-1})/\sinh \rho_i(x_i - x_{i-1}), & x_{i-1} \leqq x \leqq x_i \\ \sinh \rho_i(x_{i+1} - x)/\sinh \rho_i(x_{i+1} - x_i), & x_i \leqq x \leqq x_{i+1} \\ 0, & x \geqq x_{i+1}\,, x \leqq x_{i-1} \end{cases}$$

for $i = 1, 2, \cdots, n - 1$, and

$$r_n(x) = \begin{cases} \sinh \rho_n(x - x_{n-1})/\sinh \rho_n(x_n - x_{n-1}), & x_{n-1} \leqq x \leqq x_n \\ \exp[-\rho_n(x - x_n)], & x_n \leqq x < \infty \\ 0, & x \leqq x_{n-1}\,. \end{cases}$$

For simplicity, assume $x_{i+1} = x_i + h$, $i = 0, 1, \cdots, n - 1$. If we neglect the difference $\rho(x) - \rho_i$ on $|x - x_i| \leqq h$, the resulting patch equations are

$$\frac{-\rho_i}{\sinh(\rho_i h)}(u_{i-1}^n + u_{i+1}^n) + [2\rho_i \cdot \coth(\rho_i h)]u_i^n = (r_i, g), \qquad i = 1, 2, \cdots, n-1$$

and

$$-\frac{\rho_n \cdot u_{n-1}^n}{\sinh(\rho_n h)} + \rho_n[1 + \coth(\rho_n h)]u_n^n = (r_n, g)$$

with $u_0^n = 0$. Here the condition at infinity has been incorporated in the last equation.

II. Difference Equations for Partial Differential Equations. In Part I we discussed the possibility of deriving accurate difference approximations for Sturm-Liouville operators. Since many typical problems of mathematical physics involve the Laplace operator in some separable coordinate system it is natural to investigate the possible extentions of our methods to such problems.

II.1 Boundary Value Problems. Consider the boundary value problem

$$Lu(x, y) = f(x, y) \tag{7}$$

for a self-adjoint elliptic operator L on a domain D in the (x, y)-plane with boundary G on which, say, $u = 0$. With

$$\langle u, v\rangle = \iint_0 u(x, y)v(x, y)\, dx\, dy$$

and

$$Q(u) = \langle u, Lu\rangle - 2\langle f, u\rangle \tag{8}$$

this problem may be associated with the variational problem

$$\min_{w \in \Omega} Q(w)$$

for an admissible class Ω of smooth functions vanishing on Γ.

For purposes of deriving finite difference equations it is natural (cf. [2]) to triangulate D and extend the admissibility conditions for the variational problem by allowing continuous piecewise linear functions on the triangulated subdomains. More generally, D may be subdivided into subdomains $\{D_i\}$ with piecewise smooth boundaries $\{\Gamma_i\}$; for admissibility $w(x, y)$ may be arbitrary but continuous on every connected set of segments of Γ_i, its values on D_i being taken as the solutions of the homogeneous problem $Lu = 0$ in D_i having the assumed values of w on Γ_i. The resulting Euler equations, corresponding to equation (5), become now conditions between line integrals of $w(x, y)$ over neighboring boundary segments.

A considerable simplification results when the operator L is separable in a rectangular domain. Let

$$M = -\frac{\partial}{\partial x} p(x) \frac{\partial}{\partial x} + q(x)$$

and

$$N = -\frac{\partial}{\partial y}\hat{p}(y)\frac{\partial}{\partial y} + \hat{q}(y)$$

and suppose $L = M + N$. Introducing a lattice $x = x_i$, $y = y_j$, $i, j = 0, \pm 1, \cdots$ we may associate a patch basis $\{r_i(x)\}$ for M and a basis $\{s_j(y)\}$ for N separately and consider as an admissible class Ω_{mn} functions of the form

$$w(x, y) = \sum_{i,j} w_{ij} r_i(x) s_j(y) \tag{9}$$

where $w_{ij} = 0$ if (x_i, y_j) lies outside D. The variational problem

$$\min_{w \in \Omega_{mn}} Q(u)$$

results in the system of Euler equations

$$\sum_{k,l} w_{kl}[\langle r_i s_j, s_l M r_k\rangle + \langle r_i s_j, r_k N s_l\rangle] = \langle r_i s_j, f\rangle \qquad (x_i, y_j) \in D' \tag{10}$$

the expression on the left involving the nine points $w_{i+\mu, j+\nu}$, $\mu, \nu = 0, \pm 1$.

Unlike the one-dimensional problem, the solution $u(x, y)$ of (7) will not, in general, satisfy (10); nevertheless our previous results make it plausible that (10) affords a more accurate system of difference equations than would in general, result from straightforward differencing of (10). See [6].

The fact, also, that (10) is obtained from a variational principle provides a convenient setting for discussing gradient iterative techniques (cf. [3], [4], [5]) for approximating the solution of this system. An example is furnished by the following "alternating direction" scheme: Considering both u^k, v^k to be given by an expansion in Ω_{mn}, let

$$\begin{aligned} v^k - u^k + \lambda\phi^k &= 0 \\ u^{k+1} - v^k + \mu\psi^k &= 0 \end{aligned} \tag{11}$$

where, with $\tilde{f} = \sum_{i,j} f(x_i, y_j) r_i(x) s_j(y)$,

$$\phi^k = Mu^k - \tilde{f} + Nv^k$$

and

$$\psi^k = Nv^k - \tilde{f} + Mu^{k+1}$$

The equality in (11) is to be understood in the sense that the left hand terms are orthogonal to an arbitrary function in Ω_{mn}.

Clearly,

$$Q(v^k) = Q(u^k) - 2\lambda\langle\phi^k, Lu^k - \tilde{f}\rangle + \lambda^2\langle\phi^k, L\phi^k\rangle$$

and

$$\begin{aligned} Q(u^{k+1}) &= Q(v^k) - 2\mu\langle\psi^k, Lv^k - \tilde{f}\rangle + \mu^2\langle\psi^k, L\psi^k\rangle \\ &= Q(u^k) - 2\lambda\langle\phi^k, Lu^k - \tilde{f}\rangle + \lambda^2\langle\phi^k, L\phi^k\rangle \\ &\qquad - 2\mu\langle\psi^k, Lv^k - \tilde{f}\rangle + \mu^2\langle\psi^k, L\psi^k\rangle. \end{aligned} \tag{12}$$

Now

$$\begin{aligned}\lambda\langle\phi^k, Lu^k - \bar{f}\rangle + \mu\langle\psi^k, Lv^k - \bar{f}\rangle &= \lambda\langle\phi^k, \phi^k\rangle + \mu\langle\psi^k, \psi^k\rangle \\ &\quad + \lambda^2\langle N(v^k - u^k), \phi^k\rangle + \mu^2\langle M(u^{k+1} - v^k), \psi^k\rangle \\ &= \lambda\langle\phi^k, \phi^k\rangle + \mu\langle\psi^k, \psi^k\rangle + \lambda^2\langle N\phi^k, \phi^k\rangle + \mu^2\langle M\psi^k, \psi^k\rangle\end{aligned}$$

and, comparing with (12), we observe that the inequality

$$Q(u^{k+1}) \leqq Q(u^k)$$

may be insured by requiring, separately, the inequalities

$$\frac{\lambda}{2}\langle\phi^k, L\phi^k\rangle \leqq \langle\phi^k, \phi^k\rangle + \lambda\langle N\phi^k, \phi^k\rangle$$

and

$$\frac{\mu}{2}\langle\psi^k, L\psi^k\rangle \leqq \langle\psi^k, \psi^k\rangle + \mu\langle M\psi^k, \psi^k\rangle,$$

i.e.,

$$\begin{aligned}\lambda\langle\phi^k, M\phi^k\rangle &\leqq 2\langle\phi^k, \phi^k\rangle + \lambda\langle N\phi^k, \phi^k\rangle, \\ \mu\langle\psi^k, N\psi^k\rangle &\leqq 2\langle\psi^k, \psi^k\rangle + \mu\langle M\psi^k, \psi^k\rangle.\end{aligned} \tag{13}$$

Hence, if

$$\{\underline{\rho}, \underline{\sigma}\} = \operatorname*{g.l.b.}_{w \in \Omega_{mn}} \left\{\frac{\langle w, Mw\rangle}{\langle w, w\rangle}, \frac{\langle w, Nw\rangle}{\langle w, w\rangle}\right\}$$

$$\{\bar{\rho}, \bar{\sigma}\} = \operatorname*{l.u.b.}_{w \in \Omega_{mn}} \left\{\frac{\langle w, Mw\rangle}{\langle w, w\rangle}, \frac{\langle w, Nw\rangle}{\langle w, w\rangle}\right\}$$

these latter inequalities may be insured for all k by fixed values λ, μ satisfying

$$\begin{aligned}\lambda &\leqq \frac{2}{\bar{\rho} - \underline{\sigma}} \quad \text{and,} \\ \mu &\leqq \frac{2}{\bar{\sigma} - \underline{\rho}}.\end{aligned} \tag{14}$$

A simpler criterion, more useful in practice, results using Frobenius' estimates

$$\{\bar{\rho}, \bar{\sigma}\} \leqq \{\max_i \sum_j |(r_i, Mr_j|, \max_i \sum_j |(s_i, Ns_j)|\}$$

and

$$\{\underline{\rho}, \underline{\sigma}\} \leqq \{\min_i ||(r_i, Mr_i)| - \sum_{i \neq j} |(r_i, Mr_j)||, \min_i ||(s_i, Ns_i)| - \sum_{i \neq j} |(s_i, Ns_j)||\}.$$

We may note that, when $\langle\phi^k, M\phi^k\rangle = \langle\phi^k, N\phi^k\rangle$ as may occur, for example, when $L = -\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}\right)$, (13) is satisfied for any choice of λ, μ. The results of Lees [5] suggest that (13) may be unnecessarily restrictive in other cases also.

Finally, we may remark that if we allow the values λ, μ to be altered at each step of the iteration, the choices

$$\lambda^k = \frac{(\phi^k, \phi^k)}{(\phi^k, M\phi^k) - (\phi^k, N\phi^k)}$$

and

$$\mu^k = \frac{(\psi^k, \psi^k)}{(\psi^k, N\psi^k) - (\psi^k, M\psi^k)}$$

will serve to maximize the difference $Q(u^k) - Q(u^{k+1})$.

II.2 Parabolic Equations. In order to illustrate the treatment of initial value problems we shall consider, finally, the equation

$$\frac{\partial u(x, t)}{\partial t} + Lu(x, t) = 0, \qquad a < x < b, t > 0 \tag{16}$$

with the initial condition $u(x, 0) = u_0(x)$ and the boundary condition, say, $u(a, t) = u(b, t) = 0$.* Here $Lu = -(p(x)u_x)_x + q(x)$. Our previous discussion suggests the following, purely formal, procedure for associating difference equations with this problem: assume $u^n(x, t) \in \Omega_n$ given by

$$u^n(x, t) = \sum_{i=1}^{n} u_i^n(t) r_i(x), \tag{17}$$

where $\{r_i(x)\}$ forms a patch basis for L with respect to a given covering of (a, b) by patch intervals; then impose the conditions

$$\left(\frac{\partial u^n(t)}{\partial t} + Lu^n(t), r_i\right) = 0, \qquad i = 1, 2, \cdots, n \tag{18}$$

The resulting equations

$$\sum_{j=1}^{n} \left\{(r_i, r_j) \frac{d}{dt} u_j^n(t) + (r_i, Lr_j)u_j^n(t)\right\} = 0, \qquad i = 1, 2, \cdots, n, \tag{19}$$

a system of differential-difference equations, are to be solved with initial conditions $u_i^n(0) = u_0(x_i)$, assuming the boundary conditions have been incorporated into (19). By suitably replacing the derivative term in (19) by a difference term various "explicit" and "implicit" difference equations result. To prove the stability of the resulting difference equations (and hence their convergence) it is sufficient to show the boundness of the time growth of certain related energy norms (cf. Lees [5], [7], [8]). The following variant of the usual energy argument for (16) will serve to motivate our discussion of corresponding estimates for difference equations and indicate certain differences from Lees' treatment.

We first multiply (16) by the Green's function $K(x, y)$ for L on (a, b), integrate and note the boundary conditions to obtain the integral equation

$$\int_a^b K(\xi, x)u_t(\xi, t)\, d\xi + u(x, t) = 0 \tag{20}$$

* It will become evident, on the basis of the discussion given in Part I, that more general boundary conditions appropriate for L may be treated without essential modification.

(we have set $u_t = \partial u/\partial t$). We now multiply (20) first by $u(x, t)$ and integrate with respect to x to obtain

$$\frac{1}{2}\frac{d}{dt}(u(t), Ku(t)) + (u(t), u(t)) = 0 \tag{21}$$

where

$$(u(t), v(t)) = \int_a^b u(x, t)v(x, t)\,dx$$

and

$$(u(t), Ku(t)) = \int_a^b\int_a^b K(x, y)u(x, t)u(y, t)\,dx\,dy.$$

Similarly, we may multiply (20) instead by $u_t(x, t)$ and integrate, obtaining

$$(u_t(t), Ku_t(t)) + \frac{1}{2}\frac{d}{dt}(u(t), u(t)) = 0. \tag{22}$$

From these expressions the "energy" norm estimates

$$(u(t), Ku(t)) \leqq (u(0), Kw(0)) \tag{21$'$}$$

and

$$(u(t), u(t)) \leqq (u(0), u(0)) \tag{22$'$}$$

result, recalling that the integral kernel formed with the Green's function is positive definite.

Representing the solution $u^n(x, t) \in \Omega_n$ of the differential-difference system (18) by (17), an analogous argument yields corresponding estimates†

$$(u^n(t), K^n u^n(t)) \leqq (u^n(0), K^n u^n(0))$$

and

$$(u^n(t), u^n(t)) \leqq (u^n(0), u^n(0)).$$

For the representative "implicit" and "explicit" difference equations related to (18) by time differencing discussed below, it is the analogue of (21) which furnishes the appropriate norm estimate for the former, while (22) is appropriate for the latter.

In order to illustrate these remarks, consider first the implicit system

$$\frac{1}{\Delta t}\sum_{j=1}^{n}[\Delta v_j(t)(r_i, r_j) + v_j(t)(r_i, Lr_j)] = 0, \qquad i = 1, 2, \cdots, n \tag{23}$$

which results from (18) by replacing $du_i^n(t)/dt$ by the backward difference $\Delta u_i^n(t)/\Delta t = [u_i^n(t) - u_i^n(t - \Delta t)]/\Delta t$. Multiplying (22) by $K(x_i, x_k)$ and summing we obtain

$$\frac{1}{\Delta t}\sum_{i,j}\Delta v_i(t)(r_i, r_j)K(x_j, x_k) + v_k(t) = 0, \qquad k = 1, 2, \cdots, n \tag{24}$$

† Since $(\phi, K\phi)$ is positive definite, so also is the matrix $(K(x_i, x_j))$, and hence $(\phi^n, K^n\phi^n)$.

since $\sum_j K_{jk}(r_j, Lr_l) = \delta_{kl}$. Now, for functions $\phi(x, t)$, $\psi(x, t)$ represented by (17),

$$(\phi(t), \psi(t)) = \sum_{i,j} \phi_i(t)\psi_j(t)(r_i, r_j).$$

Hence, multiplying (24) by $(r_k, r_l)[v_l(t) + v_l(t - \Delta t)]$, summing on k, l, we obtain

$$(25)\quad \frac{1}{\Delta t}[(v(t), K^n v(t)) - (v(t - \Delta t), K^n v(t - \Delta t))] + (v(t), v(t - \Delta t)) + (v(t), v(t)) = 0$$

(compare to (21)). Now,

$$(v(t), v(t - \Delta t)) \geqq -\tfrac{1}{2}(v(t), v(t)) - \tfrac{1}{2}(v(t - \Delta t), v(t - \Delta t)).$$

If we introduce the norm

$$\| v(t) \|_{im} = \left\{\frac{1}{\Delta t}(v(t), K^n v(t)) + \frac{1}{2}(v(t), v(t))\right\}^{1/2}$$

(25) yields, finally,

$$(26)\quad \| v(t + \Delta t) \|_{im} \leqq \| v(t) \|_{im}.$$

Consider now the explicit system

$$(27)\quad \frac{\sigma}{\Delta t}\nabla w_j(t) + \sum_{i=1}^{n} w_i(t)(r_j, Lr_i) = 0, \qquad j = 1, 2, \cdots, n$$

obtained from (18) by approximating $du_i^n(t)/dt$ by the forward difference $\nabla u_i^n(t)/\Delta t = [u_i^n(t + \Delta t) - u_i^n(t)]/\Delta t$ and introducing the approximation $(r_i, r_j) = \sigma\delta_{ij}$.

We multiply (27) by K_{jk} and sum on j to obtain

$$\frac{\sigma}{\Delta t}\sum_j \nabla w_j(t)K_{jk} + w_k(t) = 0.$$

Multiplying next by $(r_k, r_l)\nabla w_l(t)$, summing over k, l and noting the relation

$$2\sum_{k,l} w_k(t)(r_l, r_l)\nabla w_l(t) = 2(w(t), \nabla w(t)) = (w(t + \Delta t), w(t + \Delta t)) - (w(t), w(t)) - (\nabla w(t), \nabla w(t))$$

we then obtain (compare to (22))

$$(28)\quad \| w(t + \Delta t) \|_{ex}^2 = \| w(t) \|_{ex}^2 - \frac{2\sigma}{\Delta t}\sum_{j,k,l} \nabla w_j(t)K(x_j, x_k)(r_k, r_l)\nabla w_l(t) + \| \nabla w(t) \|_{ex}^2$$

where

$$\| w(t) \|_{ex} = (w(t), w(t))^{1/2}.$$

Let μ denote the smallest eigenvalue of $(K(x_i, x_j))$; then

$$\sum_{j,k,l} \nabla w_j(t)K(x_j, x_k)(r_k, r_l)\nabla w_l(t) \geqq \mu\| \nabla w(t) \|_{ex}^2.$$

Hence, if we impose the stability condition

$$\frac{2\sigma\mu}{\Delta t} \geqq 1 \tag{29}$$

the estimate

$$\| w(t + \Delta t) \|_{ex} \leqq \| w(t) \|_{ex} \tag{30}$$

results.

A more useful form of the condition (29) is obtained by noticing that, because $(K(x_i, x_j))^{-1} = (r_i, Lr_j)$, an upper bound for μ^{-1} may be obtained through the estimate (Frobenius)

$$\mu^{-1} \leqq \max_i \sum_j | (r_i, Lr_j) |.$$

Thus (29) may be replaced by the simpler estimate

$$\frac{2\sigma}{\Delta t} \geqq \max_i \sum_j | (r_i, Lr_j) |. \tag{31}$$

For the heat equation $u_t = u_{xx}$, (27) assumes the form

$$\frac{\Delta x}{\Delta t} [u_i(t + \Delta t) - u_i(t)] - \frac{1}{\Delta x} [u_{i+1}(t) + u_{i-1}(t) - 2u_i(t)] = 0$$

and (cf. Example A of I.2) $\max_i \sum_j | (r_i L r_j) | = 4/\Delta x$; (31) then becomes the familiar stability condition of Courant, Friedrichs and Lewy [9], viz.,

$$\frac{1}{2} \geqq \frac{\Delta t}{\Delta x^2}.$$

We shall conclude this paper by illustrating the application of the methods discussed in this section to the following

Example D. Solve the heat equation with cylindrical symmetry

$$u_t(x, t) - \frac{1}{x} \frac{\partial}{\partial x} \left(x \frac{\partial}{\partial x} \right) u(x, t) = 0, \qquad 0 < x < 1$$

with the initial conditions

$$u(x, 0) = u_0(x), \qquad 0 < x < 1$$

and the boundary conditions

$$u(0, t) = \text{finite}, \qquad u(1, t) = 0, \qquad t > 0$$

by an explicit difference equation.

Appropriate to the present example is the inner product

$$(\phi, \psi) = \int_0^1 \phi(x)\psi(x)x \, dx.$$

The patch basis with respect to a given subdivision of (0, 1) are given by the functions

$$r_1(x) = \begin{cases} 1, & 0 \leqq x \leqq x_1 \\ (\log x/x_2)/(\log x_1/x_2), & x_1 \leqq x \leqq x_2 \\ 0, & x \leqq 0,\ x \geqq x_2 \end{cases}$$

$$r_i(x) = \begin{cases} (\log x/x_{i+1})/(\log x_i/x_{i+1}), & x_i \leqq x \leqq x_{i+1} \\ (\log x/x_{i-1})/(\log x_i/x_{i-1}), & x_{i-1} \leqq x \geqq x_i \\ 0, & x \notin (x_{i-1}, x_{i+1}) \end{cases}$$

$$i = 2, 3, \cdots, n.$$

Hence, assuming

$$w(x, t) = \sum_i w_i(t) r_i(x)$$

we obtain, with $L = -\frac{1}{x}\frac{\partial}{\partial x} x \frac{\partial}{\partial x}$,

$$(r_1, Lw(t)) = [w_2(t) - w_1(t)]/(\log x_1/x_2),$$

$$\mathrm{D}_1: \quad (r_i, Lw(t)) = [w_{i+1}(t) - w_i(t)]/(\log x_i/x_{i+1}) + [w_i(t) - w_{i-1}(t)]/(\log x_i/x_{i-1})$$

$$i = 2, 3, \cdots, n.$$

The choice of a uniform subdivision, $x_{i+1} - x_i = h$, results in the familiar approximation

$$(r_i, Lw(t)) \simeq -\frac{x_i}{h}\left[\left(1 + \frac{1}{2}\frac{h}{x_i}\right) w_{i+1}(t) + \left(1 - \frac{1}{2}\frac{h}{x_i}\right) w_{i-1}(t)\right] + \frac{2x_i}{h} w_i(t)$$

the accuracy of which is least near the origin.

Of more novel interest is the subdivision of $(0, 1)$ by the geometric sequence of points $x_{j+1} = \alpha^{j-n}$, $\alpha > 1$, $j = 0, 1, \cdots, n$. Then

$$(r_i, Lw(t)) = -\frac{1}{\log \alpha}[w_{i+1}(t) + w_{i-1}(t)] + \frac{2}{\log \alpha} w_i(t) \qquad i = 2, 3, \cdots, n$$

and

$$(r_1, Lw(t)) = -\frac{1}{\log \alpha}[w_2(t) - w_1(t)].$$

Let $\sigma_i = \frac{1}{2}(x_{i+1} - x_{i-1})x_i$ and introduce the approximation $(r_i, r_j) = \sigma_i \delta_{ij}$. Corresponding to (27) we then consider the following system of explicit difference equations:

$$\mathrm{D}_2: \quad \begin{aligned} w_j(t + \Delta t) &= w_j(t) + \frac{\Delta t}{\sigma_j \log \alpha}[w_{j+1}(t) + w_{j-1}(t) - 2w_j(t)] = 0, \qquad j = 2, 3, \cdots, n. \\ w_1(t + \Delta t) &= w_1(t) + \frac{\Delta t}{\sigma_1 \log \alpha}[w_2(t) - w_1(t)] \end{aligned}$$

subject to the initial conditions $w_j(0) = u_0(x_j)$ and the boundary condition $w_{n+1}(t) = 0$.

Unlike (27) where σ is fixed this system contains the variable σ_j. The previous discussion applies, however, providing we replace the value σ in (29) by $\sigma = \min_j \sigma_j = \alpha^{1-2n}$. The resulting stability condition (31) then takes the form

$$\Delta t \leqq \frac{\alpha^{1-2n} \log \alpha}{4}.$$

Lawrence Radiation Laboratory
University of California
Livermore, California

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