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Alternating Direction Methods for Three Space Variables

By

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1. Introduction

Alternating direction methods have proved valuable in the approximation of the solutions of parabolic and elliptic differential equations in two space variables by finite differences. Two basic methods have been introduced. The original method [*3*, *12*], when applied to the heat equation in a rectangle, is a perturbation of the Crank-Nicolson difference equation and is second order correct both in space and time. Unfortunately, the obvious generalization of this method to three space variables is not stable for a large ratio of the time increment to the square of the space increment. The second alternating direction method [*10*], again when applied to the heat equation in a rectangle, is a perturbation of the backward difference equation; consequently, it is only first order correct in time. This method can be applied to three space variable problems and was so presented in the earlier paper.

The object of this paper is to present an alternating direction method for the three space variables that is a modification of the Crank-Nicolson equation. In order to do this, the original alternating direction method will be reformulated and then generalized. Both mildly nonlinear parabolic and elliptic problems with boundary values specified on the boundary of a rectangular parallelepiped will be considered. *All theorems in this paper are proved under the restriction that the region is a cube, and this hypothesis will be omitted in the statement of the theorems.* Clearly, the results remain valid for an arbitrary interval.

In the parabolic case, the differential equation will be of the form

$$u_{xx} + u_{yy} + u_{zz} = u_t + \varphi(x, y, z, t, u). \tag{1.1}$$

The case in which φ is independent of u will be treated first, and it will be shown that the error is $O\big((\Delta x)^2 + (\Delta t)^2\big)$ if the solution of the differential equation is sufficiently smooth. If the method is applied directly to the nonlinear equation with φ being evaluated at the known time level, the accuracy drops to $O\big((\Delta x)^2 + \Delta t\big)$; however, if a predictor-corrector generalization of the method is used, the higher accuracy is recovered. An extrapolation to the limit will also be considered, and the calculational effort will be estimated for each of these problems. A generalization of (1.1) to a simple parabolic system will also be treated.

In the elliptic case the differential equation will correspond to (1.1); i.e.,

$$u_{xx} + u_{yy} + u_{zz} = \varphi(x, y, z, u). \tag{1.2}$$

Again the case where φ does not depend on u will be treated first; the iterative technique will prove to be an improvement over the procedure of [*10*]. The nonlinear problem will be treated two ways. First, a direct application of the technique will be studied; under a restriction on

$$\left|\frac{\partial \varphi}{\partial u}\right|$$

that is somewhat too strong, a proof will be given that the iteration converges using a variable sequence of parameters (indeed, the same sequence as for Laplace's equation) and, moreover, requires the same $O\left((\Delta x)^{-3}\log(\Delta x)^{-1}\right)$ calculations that characterize the computing requirements for alternating direction methods for Laplace's equation. Then, an indirect method [7] using a Picard type outer iteration and alternating direction inner iteration will be considered. Under more natural conditions on φ, the iteration will again be shown to be convergent and to lead to $O\left((\Delta x)^{-3}\log(\Delta x)^{-1}\right)$ calculations; however, the multiplier should be expected to be larger in this case.

Generalizations of the method as it would apply to more complex parabolic and elliptic equations will be outlined. At the moment proofs are lacking in these cases; however, it is hoped that the recent results of LEES [11] can be extended to cover these applications.

The results presented here were presented in abstract form earlier [9]; most were known to the author five years ago. The method to be discussed has recently been discovered independently by BRIAN [2]; however, he did not discuss convergence proofs.

2. Reformulation of Alternating Direction Methods

Consider the original alternating direction method for the heat equation in two space variables:

$$\text{(2.1)}\quad \begin{aligned} &\text{(a)} \qquad \Delta_x^2 w_{i,j,n+\frac12} + \Delta_y^2 w_{ijn} = \frac{w_{i,j,n+\frac12} - w_{ijn}}{\frac12 \Delta t},\\ &\text{(b)} \qquad \Delta_x^2 w_{i,j,n+\frac12} + \Delta_y^2 w_{i,j,n+1} = \frac{w_{i,j,n+1} - w_{i,j,n+\frac12}}{\frac12 \Delta t}, \end{aligned}$$

where

$$\text{(2.2)}\quad \begin{gathered} x_i = i\,\Delta x, \qquad y_j = j\,\Delta x, \qquad t_n = n\,\Delta t, \qquad w_{ijn} = w(x_i, y_j, t_n),\\ \Delta_x^2 w_{ijn} = (w_{i+1,j,n} - 2w_{ijn} + w_{i-1,j,n})/(\Delta x)^2. \end{gathered}$$

On a rectangular region the intermediate values $w_{i,j,n+\frac12}$ can easily be eliminated to obtain an equation relating the solution at t_{n+1} to that at t_n. Subtracting (2.1 a) from (2.1 b), we obtain

$$\text{(2.3)}\qquad w_{n+\frac12} = \frac12 (w_{n+1} + w_n) - \frac{\Delta t}{4}\, \Delta_y^2 (w_{n+1} - w_n),$$

where the i and j indices have been suppressed. If (2.3) is substituted into (2.1), it follows that

$$\text{(2.4)}\qquad \frac12 (\Delta_x^2 + \Delta_y^2)(w_{n+1} + w_n) = \frac{w_{n+1} - w_n}{\Delta t} + \frac{\Delta t}{4}\, \Delta_x^2 \Delta_y^2 (w_{n+1} - w_n).$$

Note that (2.4) is almost the Crank-Nicolson equation, the only difference being an additional term. This term should tend to zero like $(\Delta t)^2$ for sufficiently smooth solutions; and it is easy to prove [8] that the overall truncation error for (2.4) behaves like $O\big((\Delta t)^2+(\Delta x)^2\big)$.

Let us see if we can find another way of obtaining (2.4) by an alternating direction difference equation. What we are trying to do is to factor the operator giving the Crank-Nicolson equation,

$$\frac{1}{2}\left(\Delta_x^2+\Delta_y^2\right)\left(w_{n+1}+w_n\right)=\frac{w_{n+1}-w_n}{\Delta t}, \tag{2.5}$$

into a product of two operators. First, move forward in time in the x-term:

$$\frac{1}{2}\Delta_x^2\left(w_{n+1}^*+w_n\right)+\Delta_y^2 w_n=\frac{w_{n+1}^*-w_n}{\Delta t}. \tag{2.6a}$$

Then, correct the relation by moving forward in time in the y-term:

$$\frac{1}{2}\Delta_x^2\left(w_{n+1}^*+w_n\right)+\frac{1}{2}\Delta_y^2\left(w_{n+1}+w_n\right)=\frac{w_{n+1}-w_n}{\Delta t}. \tag{2.6b}$$

The second equation, (2.6b), is again almost the Crank-Nicolson equation, excepting only the w_{n+1}^* term. The system (2.6) is an alternating direction procedure with no worse than tridiagonal linear equations to be solved at each time step. Let us eliminate w_{n+1}^* to obtain the difference equation for w_{n+1} in terms of w_n. By subtracting (2.6a) from (2.6b), we find that

$$w_{n+1}^*=w_{n+1}-\frac{\Delta t}{2}\Delta_y^2\left(w_{n+1}-w_n\right). \tag{2.7}$$

Upon substituting w_{n+1}^* into (2.6b), we find that (2.4) is again satisfied; consequently, the difference systems (2.1) and (2.6) are equivalent on a rectangle.

3. The Parabolic Difference Equation for the Heat Equation

The method of (2.6) can easily be generalized to an arbitrary number of dimensions. Consider the heat equation with three space variables. Obtain a first estimate of the solution at time t_{n+1} by evaluating half of the second difference with respect to x at t_{n+1}:

$$\frac{1}{2}\Delta_x^2\left(w_{n+1}^*+w_n\right)+\Delta_y^2 w_n+\Delta_z^2 w_n=\frac{w_{n+1}^*-w_n}{\Delta t}. \tag{3.1a}$$

Then, move half of the evaluation of the other second differences forward successively:

$$\frac{1}{2}\Delta_x^2\left(w_{n+1}^*+w_n\right)+\frac{1}{2}\Delta_y^2\left(w_{n+1}^{**}+w_n\right)+\Delta_z^2 w_n=\frac{w_{n+1}^{**}-w_n}{\Delta t}, \tag{3.1b}$$

$$\frac{1}{2}\Delta_x^2\left(w_{n+1}^*+w_n\right)+\frac{1}{2}\Delta_y^2\left(w_{n+1}^{**}+w_n\right)+\frac{1}{2}\Delta_z^2\left(w_{n+1}+w_n\right)=\frac{w_{n+1}-w_n}{\Delta t}. \tag{3.1c}$$

The stability and convergence of the difference system (3.1) for the boundary value problem for the heat equation on a cubic region will be established shortly, and the system will later be applied as an iterative method for Laplace's equation. Before considering these points, let us look at the algebraic problem arising in the evaluation of (3.1) at each time step. The algebraic equations for w_{n+1}^{**} and w_{n+1} can be simplified by subtracting (3.1a) from (3.1b) and (3.1b) from

(3.1 c), respectively. After rearrangement, the resulting equations become

$$\text{(3.2)}\quad \begin{aligned} &\text{(a)} \quad \left(\Delta_x^2 - \frac{2}{\Delta t}\right) w_{n+1}^* = -\left(\Delta_x^2 + 2\Delta_y^2 + 2\Delta_z^2 + \frac{2}{\Delta t}\right) w_n, \\ &\text{(b)} \quad \left(\Delta_y^2 - \frac{2}{\Delta t}\right) w_{n+1}^{**} = \Delta_y^2 w_n - \frac{2}{\Delta t} w_{n+1}^*, \\ &\text{(c)} \quad \left(\Delta_z^2 - \frac{2}{\Delta t}\right) w_{n+1} = \Delta_z^2 w_n - \frac{2}{\Delta t} w_{n+1}^{**}. \end{aligned}$$

It is clear that the evaluation of w_{n+1} consists of solving tridiagonal linear equations, a simple operation, three times.

4. Stability and Convergence for the Parabolic Problem

When the region is a cube (or a rectangular parallelepiped), the intermediate solutions w_{n+1}^* and w_{n+1}^{**} can be eliminated, using the last two relations of (3.2). The resulting difference equation is

$$\text{(4.1)}\quad \begin{aligned} &(\Delta_x^2 + \Delta_y^2 + \Delta_z^2)(w_{n+1} + w_n) = 2\,\frac{w_{n+1} - w_n}{\Delta t} + \\ &+ \frac{\Delta t}{2}(\Delta_x^2\Delta_y^2 + \Delta_y^2\Delta_z^2 + \Delta_z^2\Delta_x^2)(w_{n+1} - w_n) - \left(\frac{\Delta t}{2}\right)^2 \Delta_x^2\Delta_y^2\Delta_z^2(w_{n+1} - w_n). \end{aligned}$$

Note that (4.1) is, as expected, a perturbation of the Crank-Nicolson difference equation. Let us consider the application of (4.1) to the boundary value problem:

$$\text{(4.2)}\quad \begin{aligned} u_{xx} + u_{yy} + u_{zz} &= u_t, & (x, y, z, t) &\in R \times (0, T], \\ u(x, y, z, 0) &= f(x, y, z), & (x, y, z, t) &\in R \times \{0\}, \\ u(x, y, z, t) &= g(x, y, z, t), & (x, y, z, t) &\in \partial R \times (0, T], \end{aligned}$$

where R is the cube $0 < x, y, z < 1$ and ∂R its boundary. The data f and g should be assigned to w on the boundary:

$$\text{(4.3)}\quad \begin{aligned} w_{i,j,k,0} &= f_{i,j,k}, & (x_i, y_j, z_k, 0) &\in R \times \{0\}, \\ w_{i,j,k,n} &= g_{i,j,k,n}, & (x_i, y_j, z_k, t_n) &\in \partial R \times (0, T). \end{aligned}$$

Now, consider the analysis of the discretization error induced by using (3.2), (4.3). First, let us assume that a solution u of (4.2) exists and, moreover, that u has bounded derivatives of sixth order in $R \times [0, T]$. Then, it can be shown that

$$\text{(4.4)}\quad \begin{aligned} &(\Delta_x^2 + \Delta_y^2 + \Delta_z^2)(u_{n+1} + u_n) = 2\,\frac{u_{n+1} - u_n}{\Delta t} + \\ &+ \frac{\Delta t}{2}(\Delta_x^2\Delta_y^2 + \Delta_y^2\Delta_z^2 + \Delta_z^2\Delta_x^2)(u_{n+1} - u_n) - \left(\frac{\Delta t}{2}\right)^2 \Delta_x^2\Delta_y^2\Delta_z^2(u_{n+1} - u_n) + 2e_n, \end{aligned}$$

where

$$\text{(4.5)}\quad e_{ijkn} = O\left((\Delta t)^2 + (\Delta x)^2\right), \qquad 0 \leqq t_n \leqq T,$$

since the perturbation terms are both $O\left((\Delta t)^2 + (\Delta x)^2\right)$ when $u \in C^6$. Let

$$\text{(4.6)}\quad \alpha = u - w$$

represent the discretization error. Then,

$$(\Delta_x^2+\Delta_y^2+\Delta_z^2)(\alpha_{n+1}+\alpha_n)=2\,\frac{\alpha_{n+1}-\alpha_n}{\Delta t}+$$

$$+\frac{\Delta t}{2}(\Delta_x^2\Delta_y^2+\Delta_y^2\Delta_z^2+\Delta_z^2\Delta_x^2)(\alpha_{n+1}-\alpha_n)-\left(\frac{\Delta t}{2}\right)^2\Delta_x^2\Delta_y^2\Delta_z^2(\alpha_{n+1}-\alpha_n)+2e_n, \tag{4.7}$$

$$\alpha=0, \qquad (x,y,z,t)\in(R\times\{0\})\cup(\partial R\times(0,T]).$$

The estimation of α can be facilitated by the following lemma.

Lemma 1. Let

$$(\Delta_x^2+\Delta_y^2+\Delta_z^2)(\zeta_1+\zeta_0)=2\,\frac{\zeta_1-\zeta_0}{\Delta t}+\frac{\Delta t}{2}(\Delta_x^2\Delta_y^2+\Delta_y^2\Delta_z^2+\Delta_z^2\Delta_x^2)(\zeta_1-\zeta_0)-$$

$$-\left(\frac{\Delta t}{2}\right)^2\Delta_x^2\Delta_y^2\Delta_z^2(\zeta_1-\zeta_0)+2e, \quad (x_i,y_j,z_k)\in R, \tag{4.8}$$

$$\zeta_1=\zeta_0=0, \qquad (x_i,y_j,z_k)\in\partial R.$$

Then,

$$\|\zeta_1\|\leqq\|\zeta_0\|+\|e\|\Delta t, \tag{4.9}$$

where

$$\|\zeta\|=\Big[\sum_{(x,y,z)\in R}\zeta_{ijk}^2(\Delta x)^3\Big]^{\frac{1}{2}}. \tag{4.10}$$

Proof. Let

$$\zeta_\mu=\sum_{p,q,r=1}^{M-1}c_{pqr}\sin\pi p x\sin\pi q y\sin\pi r z, \qquad \mu=0,1, \qquad M=(\Delta x)^{-1},$$

$$e=\sum_{p,q,r=1}^{M-1}e_{pqr}\sin\pi p x\sin\pi q y\sin\pi r z. \tag{4.11}$$

It is easy to see by direct substitution into (4.8) that

$$c_{pqr}^1=\varrho_{pqr}c_{pqr}^0+v_{pqr}e_{pqr}\Delta t, \tag{4.12}$$

where

$$X_p=\frac{2\Delta t}{(\Delta x)^2}\sin^2\frac{\pi p\Delta x}{2},$$

$$\varrho_{pqr}=\frac{1-(X_p+X_q+X_r)+(X_pX_q+X_qX_r+X_rX_p)+X_pX_qX_r}{1+(X_p+X_q+X_r)+(X_pX_q+X_qX_r+X_rX_p)+X_pX_qX_r}, \tag{4.13}$$

$$v_{pqr}=-[1+(X_p+X_q+X_r)+(X_pX_q+X_qX_r+X_rX_p)+X_pX_qX_r]^{-1}.$$

Thus, for any positive time step,

$$|\varrho_{pqr}|<1, \qquad |v_{pqr}|<1. \tag{4.14}$$

Consequently, by the Parseval identity,

$$\|\zeta_1\|\leqq\|\zeta_0\|+\|e\|\Delta t. \tag{4.15}$$

Let us apply this lemma to α_n. It follows from (4.7) that

$$\|\alpha_{n+1}\|\leqq\|\alpha_n\|+\|e_n\|\Delta t, \qquad n=0,1,\ldots. \tag{4.16}$$

As $\|\alpha_0\|=0$,

$$\|\alpha_n\|\leqq\sum_{k=0}^{n-1}\|e_k\|\Delta t=O\left((\Delta x)^2+(\Delta t)^2\right), \qquad 0\leqq t_n\leqq T. \tag{4.17}$$

Thus, the solution of the difference equation (3.2), (4.3) converges in the mesh L_2 norm on R with the discretization error being second order in space and time; if multi-linear interpolation is applied to the solution [5], the integral L_2 error is also $O\left((\Delta x)^2+(\Delta t)^2\right)$.

Theorem 1. If a solution u of (4.2) having bounded derivatives of the sixth order exists, the multi-linearly interpolated solution w of (3.2), (4.3) converges in the integral L_2 norm to u with an $O\left((\Delta x)^2+(\Delta t)^2\right)$ discretization error.

An asymptotic, order estimate of the calculation required to approximate u can be obtained by the procedure used in [4].

Lemma 2. Let C denote the total calculation required to advance the solution to time T and let E denote the global discretization error. If

$$\begin{aligned} C &\sim (\Delta x)^{-\alpha}(\Delta t)^{-\beta}, \\ E &\sim (\Delta x)^{\gamma}+(\Delta t)^{\delta}, \\ \Delta t &\sim (\Delta x)^{\eta}, \end{aligned} \tag{4.18}$$

as E and $\Delta x \to 0$, then the best choice of η is

$$\eta=\gamma/\delta \tag{4.19}$$

and

$$C_{\min}\sim E^{-(\alpha/\gamma+\beta/\delta)}. \tag{4.20}$$

Proof. As $\Delta t \sim (\Delta x)^{\eta}$,

$$C\sim(\Delta x)^{-(\alpha+\beta\eta)} \quad \text{and} \quad E\sim(\Delta x)^{\gamma}+(\Delta x)^{\delta\eta}.$$

If $\gamma \leqq \delta\eta$, $E\sim(\Delta x)^{\gamma}$ and $\Delta x\sim E^{1/\gamma}$. Thus,

$$C\sim E^{-(\alpha+\beta\eta)/\gamma}, \qquad \gamma\leqq\delta\eta.$$

If $\gamma\geqq\delta\eta$, $E\sim(\Delta x)^{\delta\eta}$ and $\Delta x\sim E^{1/\delta\eta}$. In this case,

$$C\sim E^{-(\alpha+\beta\eta)/\delta\eta}, \qquad \gamma\geqq\delta\eta.$$

The minimum calculation is achieved asymptotically by choosing η to maximize the exponent on E. This is easily seen to result in the conclusions of the lemma.

For the difference system (3.2), (4.3),

$$\begin{aligned} C &\sim (\Delta x)^{-3}(\Delta t)^{-1}, \\ E &\sim (\Delta x)^{2}+(\Delta t)^{2}. \end{aligned} \tag{4.21}$$

Thus, the best choice of η is

$$\eta=1, \tag{4.22}$$

and

$$C_{\min}\sim E^{-2}. \tag{4.23}$$

It can be shown readily that

$$C_{\min}\sim E^{-\frac{5}{2}} \tag{4.24}$$

for the standard explicit difference analogue of the heat equation. Consequently, as E tends to zero, considerably less computation is required to obtain an accurate approximation by this alternating direction method than by the commonly used explicit method. Improvements will be discussed shortly.

5. Mildly Nonlinear Parabolic Equations

Let us consider the generalization of (4.2) in which the differential equation is the mildly nonlinear parabolic equation

$$u_{xx} + u_{yy} + u_{zz} = u_t + \varphi(x, y, z, t, u). \tag{5.1}$$

The simplest extension of the difference system (3.2) is

$$\left(\Delta_x^2 - \frac{2}{\Delta t}\right) w_{n+1}^* = -\left(\Delta_x^2 + 2\Delta_y^2 + 2\Delta_z^2 + \frac{2}{\Delta t}\right) w_n + 2\varphi_n, \tag{5.2}$$

where

$$\varphi_n = \varphi(x_i, y_j, z_k, t_{n+\frac{1}{2}}, w_{ijkn}), \tag{5.3}$$

followed by the same last two equations of (3.2). The algebraic equations remain linear and tridiagonal. Assume that

$$|\varphi_u| \leqq B. \tag{5.4}$$

Then, the error equation (4.4) is unaltered except for the definition of e, which becomes

$$\begin{aligned} e_{ijkn} &= \varphi(x_i, y_j, z_k, t_{n+\frac{1}{2}}, u_{i,j,k,n+\frac{1}{2}}) - \varphi(x_i, y_j, z_k, t_{n+\frac{1}{2}}, w_{ijkn}) + \\ &\quad + O\left((\Delta x)^2 + (\Delta t)^2\right) = O\left(\alpha_{ijkn} + \Delta t + (\Delta x)^2\right), \end{aligned} \tag{5.5}$$

as

$$\varphi(u_{n+\frac{1}{2}}) - \varphi(w_n) = \varphi_u \cdot \left[(u_{n+\frac{1}{2}} - u_n) + (u_n - w_n)\right]. \tag{5.6}$$

By the a priori estimate

$$\begin{aligned} \|\alpha_{n+1}\| &\leqq \|\alpha_n\| + A\left[\|\alpha_n\| + \Delta t + (\Delta x)^2\right] \Delta t \\ &= (1 + A\,\Delta t)\,\|\alpha_n\| + A\left[\Delta t + (\Delta x)^2\right] \Delta t. \end{aligned} \tag{5.7}$$

As $\|\alpha_0\| = 0$,

$$\|\alpha_n\| = O\left(\Delta t + (\Delta x)^2\right). \tag{5.8}$$

Theorem 2. If (5.4) holds, the solution of (5.2), (3.2b), (3.2c), (4.3) converges with an L_2 error that is $O\left((\Delta x)^2 + \Delta t\right)$ under the same smoothness conditions as required for the case of the heat equation.

Note that the evaluation of φ at w_n causes a loss in accuracy in the time direction. Some time ago the author [6] introduced a method of predicting the value of u at the mid-time to preserve the accuracy of the Crank-Nicolson equation for a nonlinear parabolic equation, but the argument offered to support the procedure was almost wholly in error. However, let us consider using the idea with a different argument.

Assume that the solution is known up to time t_n. Then use the above process ((5.2), (3.2b), (3.2c), (4.3)) with Δt replaced by $\frac{1}{2}\Delta t$ to obtain a first estimate $\hat{w}_{n+\frac{1}{2}}$. Then, use the difference system (5.2), (3.2b), (3.2c) with φ_n replaced by

$$\hat{\varphi}_n = \varphi(x_i, y_j, z_k, t_{n+\frac{1}{2}}, \hat{w}_{i,j,k,n+\frac{1}{2}}). \tag{5.9}$$

Note that this procedure is essentially an example of the predictor-corrector methods that are familiar in the numerical solution of ordinary differential equations.

Let us consider the error. The local disturbance e becomes

$$\begin{aligned} e_{ijk} &= \varphi(x_i, y_j, z_k, t_{n+\frac{1}{2}}, u_{i,j,k,n+\frac{1}{2}}) - \varphi(x_i, y_j, z_k, t_{n+\frac{1}{2}}, \hat{w}_{i,j,k,n+\frac{1}{2}}) + \\ &+ O\left((\Delta x)^2 + (\Delta t)^2\right) = O\left(\hat{\alpha}_{i,j,k,n+\frac{1}{2}} + (\Delta x)^2 + (\Delta t)^2\right), \end{aligned} \tag{5.10}$$

where

$$\hat{\alpha}_{n+\frac{1}{2}} = u_{n+\frac{1}{2}} - \hat{w}_{n+\frac{1}{2}}. \tag{5.11}$$

Since no shifting in time is necessary in the evaluation of u, the local error maintains the desired second order correctness in the time direction. By (5.7),

$$\|\hat{\alpha}_{n+\frac{1}{2}}\| \leqq (1 + \tfrac{1}{2} A\,\Delta t)\,\|\alpha_n\| + \tfrac{1}{2} A[\Delta t + (\Delta x)^2]\,\Delta t, \tag{5.12}$$

and by the a priori estimate

$$\begin{aligned} \|\alpha_{n+1}\| &\leqq \|\alpha_n\| + A\left[\|\hat{\alpha}_{n+\frac{1}{2}}\| + (\Delta t)^2 + (\Delta x)^2\right]\Delta t \\ &\leqq (1 + B\,\Delta t)\,\|\alpha_n\| + B[(\Delta t)^2 + (\Delta x)^2]\,\Delta t. \end{aligned} \tag{5.13}$$

Consequently,

$$\|\alpha_n\| = O\left((\Delta t)^2 + (\Delta x)^2\right)$$

under the same hypotheses as before.

Theorem 3. Under the same hypotheses as for Theorem 1, the solution of the system (5.2), (3.2b), (3.2c), (4.3) using the values $\hat{w}_{n+\frac{1}{2}}$ in the evaluation of φ converges with an L_2 error that is $O\left((\Delta x)^2 + (\Delta t)^2\right)$.

Note that the arithmetic per time step is doubled by the use of the predictor; however, the increase in accuracy easily justifies this work. The estimate (4.23) remains valid with the predictor. Without it, the exponent would become $-\frac{5}{2}$.

Also, if the u_t term is replaced by $a u_t$, where a is a constant, it is clear that the same results hold after the obvious modification of the difference equation is made.

6. Mildly Nonlinear Parabolic Systems

Parabolic systems of the form

$$a_\eta u_t^\eta = u_{xx}^\eta + u_{yy}^\eta + u_{zz}^\eta + \varphi^\eta(x, y, z, t, u^1, \ldots, u^m), \qquad \eta = 1, \ldots, m, \tag{6.1}$$

where $a_1, \ldots, a_m$ are positive constants, arise from several physical problems. The alternating direction method with prediction can easily be extended to (6.1) by simply applying the above procedure to each component w^η with $2a_\eta/\Delta t$ replacing $2/\Delta t$ in the η-th equation and

$$\begin{aligned} \varphi_n^\eta &= \varphi^\eta(x_i, y_j, z_k, t_{n+\frac{1}{2}}, w_{ijkn}^1, \ldots, w_{ijkn}^m), \\ \hat{\varphi}_n^\eta &= \varphi^\eta(x_i, y_j, z_k, t_{n+\frac{1}{2}}, \hat{w}_{i,j,k,n+\frac{1}{2}}^1, \ldots, \hat{w}_{i,j,k,n+\frac{1}{2}}^m), \end{aligned} \tag{6.2}$$

replacing φ_n and $\hat{\varphi}_n$. The analysis parallels the above argument down to the stage at which $\|\alpha_{n+1}^\eta\|$ is estimated:

$$\|\alpha_{n+1}^\eta\| \leqq (1 + B\,\Delta t)\,\|\alpha_n^\eta\| + B\left[\sum_{\mu=1}^m \|\alpha_n^\mu\| + (\Delta t)^2 + (\Delta x)^2\right]\Delta t. \tag{6.3}$$

Let

$$\|\alpha_n\| = \sum_{\eta=1}^{m} \|\alpha_n^\eta\|; \tag{6.4}$$

then,

$$\|\alpha_{n+1}\| \leqq (1 + B\,\Delta t)\,\|\alpha_n\| + m\,B\left[\|\alpha_n\| + (\Delta t)^2 + (\Delta x)^2\right]\Delta t \tag{6.5}$$

and

$$\|\alpha_n\| = O\left((\Delta t)^2 + (\Delta t)^2\right). \tag{6.6}$$

Theorem 4. Under the same smoothness assumptions on the solution $u^1, \ldots, u^m$ of the system (6.1) as on the solution of the single equation (4.2), the solution of the difference system with prediction converges with an L_2 error that is $O\left((\Delta x)^2 + (\Delta t)^2\right)$.

7. Extrapolation to the Limit

BATTEN [*1, 8*] has introduced a method of extrapolation for solutions of certain difference analogues of parabolic equations. Let us consider applying the method here. After some messy calculations it can be shown that

$$e_{ijkn} = A(x_i, y_j, z_k, t_{n+\frac{1}{2}})\,(\Delta x)^2 + B(x_i, y_j, z_k, t_{n+\frac{1}{2}})\,(\Delta t)^2 + O\left((\Delta x)^4 + (\Delta t)^3\right) \tag{7.1}$$

for the linear case

$$\varphi = \varphi(x, y, z, t) \tag{7.2}$$

if $u \in C^{10}$. Both A and B are rather complex combinations of derivatives of u. Let v^* and v^{**} be the solutions of

$$\begin{aligned} v^*_{xx} + v^*_{yy} + v^{**}_{zz} &= v^*_t + A(x, y, z, t), \\ v^{**}_{xx} + v^{**}_{yy} + v^{**}_{zz} &= v^{**}_t + B(x, y, z, t), \end{aligned} \tag{7.3}$$

that vanish initially and on the boundary. Assume that v^* and v^{**} have bounded sixth derivatives. Then,

$$\begin{aligned} (\Delta_x^2 + \Delta_y^2 + \Delta_z^2)\,(v^*_{n+1} + v^*_n) &= 2\,\frac{v^*_{n+1} - v^*_n}{\Delta t} + \frac{\Delta t}{2}\,(\Delta_x^2\Delta_y^2 + \Delta_y^2\Delta_z^2 + \Delta_t^2\Delta_x^2) \times \\ &\times (v^*_{n+1} - v^*_n) - \left(\frac{\Delta t}{2}\right)^2 \Delta_x^2\Delta_y^2\Delta_z^2\,(v^*_{n+1} - v^*_n) + 2A_{n+\frac{1}{2}} + e^*_n, \end{aligned} \tag{7.4}$$

where

$$e^*_n = O\left((\Delta x)^2 + (\Delta t)^2\right). \tag{7.5}$$

A similar expression holds for v^{**}_n with B replacing A and

$$e^{**}_n = O\left((\Delta x)^2 + (\Delta t)^2\right). \tag{7.6}$$

Now, consider

$$\beta_n = \alpha_n - v^*_n\,(\Delta x)^2 - v^{**}_n(\Delta t)^2. \tag{7.7}$$

It is easy to see that β satisfies the error equation (4.7) with e_n replaced by

$$e_n(\beta) = O\left((\Delta x)^4 + (\Delta t)^3\right). \tag{7.8}$$

Consequently,

$$\|\beta_n\| = O\left((\Delta x)^4 + (\Delta t)^3\right). \tag{7.9}$$

Let us indicate the dependence of v, α, and β on t, Δx, and Δt as follows:

$$w = w(t, \Delta x, \Delta t), \qquad \alpha = \alpha(t, \Delta x, \Delta t), \qquad \beta = \beta(t, \Delta x, \Delta t). \tag{7.10}$$

The dependence of x, y, z will not be displayed. Thus,

$$\alpha(t, \Delta x, \Delta t) = v^*(t)(\Delta x)^2 + v^{**}(t)(\Delta t)^2 + \beta(t, \Delta x, \Delta t). \tag{7.11}$$

Consider the linear combination

$$W(t) = c_1 w(t, \Delta x, \Delta t) + c_2 w(t, \Delta x, \Delta t/2) + c_3 w(t, \Delta x/2, \Delta t), \tag{7.12}$$

which is defined at the points $(i\Delta x, j\Delta x, k\Delta x, n\Delta t)$, and let

$$\gamma(t) = u(t) - W(t). \tag{7.13}$$

If

$$c_1 + c_2 + c_3 = 1, \tag{7.14}$$

then

$$\begin{aligned} \gamma(t) &= c_1 \alpha(t, \Delta x, \Delta t) + c_2 \alpha(t, \Delta x, \Delta t/2) + c_3 \alpha(t, \Delta x/2, \Delta t) \\ &= (c_1 + c_2 + \tfrac{1}{4}c_3) v^*(t)(\Delta x)^2 + (c_1 + \tfrac{1}{4}c_2 + c_3) v^{**}(t)(\Delta t)^2 + \\ &\quad + c_1 \beta(t, \Delta x, \Delta t) + c_2 \beta(t, \Delta x, \Delta t/2) + c_3 \beta(t, \Delta x/2, \Delta t). \end{aligned} \tag{7.15}$$

Thus, if

$$\begin{aligned} c_1 + c_2 + c_3 &= 1, \\ c_1 + c_2 + \tfrac{1}{4}c_3 &= 0, \\ c_1 + \tfrac{1}{4}c_2 + c_3 &= 0, \end{aligned} \tag{7.16}$$

the leading terms on the error disappear, and $\gamma(t)$ would satisfy

$$\|\gamma(t)\| = O\left((\Delta x)^4 + (\Delta t)^3\right). \tag{7.17}$$

The solution of (7.16) is

$$c_1 = -\tfrac{5}{3}, \qquad c_2 = c_3 = \tfrac{4}{3}. \tag{7.18}$$

Of course, more computing is required to evaluate $W(t)$ than is required for $w(t, \Delta x, \Delta t)$. In fact, since $w(t, \Delta x, \Delta t/2)$ requires twice that for $w(t, \Delta x, \Delta t)$ and $w(t, \Delta x/2, \Delta t)$ eight times, the evaluation of $W(t)$ requires eleven times the effort that is needed for $w(t, \Delta x, \Delta t)$ for the same choice of Δx and Δt. Fortunately, the increase in accuracy leads to the use of considerably larger Δx and Δt. As

$$\begin{aligned} C &\sim (\Delta x)^{-3}(\Delta t)^{-1}, \\ E &\sim (\Delta x)^4 + (\Delta t)^3, \end{aligned} \tag{7.19}$$

for $W(t)$, the best choice of η is

$$\eta = \tfrac{4}{3}, \tag{7.20}$$

and

$$C_{\min} \sim E^{-\frac{13}{12}}. \tag{7.21}$$

The almost halving of the exponent indicates a very significant reduction in the total computing effort.

Theorem 5. Let

$$W(t) = -\tfrac{5}{3}\, w(t, \Delta x, \Delta t) + \tfrac{4}{3}\, w(t, \Delta x, \Delta t/2) + \tfrac{4}{3}\, w(t, \Delta x/2, \Delta t). \tag{7.22}$$

If $u \in C^{10}$ and $v^*, v^{**} \in C^6$, then $W(t)$ converges to $u(x, y, z, t)$ with an L_2 error that is $O\left((\Delta x)^4 + (\Delta t)^3\right)$, and

$$C_{\min} \sim E^{-\frac{13}{12}}$$

as the discretization error E tends to zero.

8. Iterative Procedure for Laplace's Equation

Let us now turn our attention to the use of the alternating direction method as an iterative technique for elliptic difference equations. We shall consider first the Laplace difference equation on the unit cube. Let

$$\begin{aligned} (\Delta_x^2 + \Delta_y^2 + \Delta_z^2)\, w_{ijk} &= \varphi_{ijk}, \qquad (x_i, y_j, z_k) \in R, \\ w_{ijk} &= g_{ijk}, \qquad (x_i, y_j, z_k) \in \partial R, \end{aligned} \tag{8.1}$$

where φ is independent of u. Let $w_{i,j,k,0}$ be arbitrary, except on ∂R where it should agree with $g_{i,j,k}$. Then, iterate by

$$\begin{aligned} (\Delta_x^2 - c_n)\, w_{n+1}^* &= -(\Delta_x^2 + 2\Delta_y^2 + 2\Delta_z^2 + c_n)\, w_n + 2\varphi, \\ (\Delta_y^2 - c_n)\, w_{n+1}^{**} &= \Delta_y^2 w_n - c_n\, w_{n+1}^*, \\ (\Delta_z^2 - c_n)\, w_{n+1} &= \Delta_z^2 w_n - c_n\, w_{n+1}^{**}, \end{aligned} \tag{8.2}$$

where the boundary values for w_{n+1}^*, w_{n+1}^{**}, and w_{n+1} are maintained equal to g and $\{c_n\}$ is a sequence of positive constants to be chosen later. Let

$$\alpha_n = w - w_n \tag{8.3}$$

denote the error in the approximate solution w_n of the algebraic equations (8.1). Note that α_n is not related to the discretization error caused by replacing the differential equation by (8.1). Then,

$$\begin{aligned} (\Delta_x^2 - c_n)\, \alpha_{n+1}^* &= -(\Delta_x^2 + 2\Delta_y^2 + 2\Delta_z^2 + c_n)\, \alpha_n, \\ (\Delta_y^2 - c_n)\, \alpha_{n+1}^{**} &= \Delta_y^2 \alpha_n - c_n\, \alpha_{n+1}^*, \\ (\Delta_z^2 - c_n)\, \alpha_{n+1} &= \Delta_z^2 \alpha_n - c_n\, \alpha_{n+1}^{**}, \end{aligned} \tag{8.4}$$

and α_{n+1}^*, α_{n+1}^{**}, and α_{n+1} vanish on ∂R.

If the parameter c_n is fixed as a positive number, it follows from (4.13) and (4.14) that

$$\|\alpha_{n+1}\| \leq \varrho \|\alpha_n\|, \tag{8.5}$$

where

$$0 < \varrho < 1. \tag{8.6}$$

Thus, the solution of (8.2) converges to the solution of (8.1) as $n \to \infty$ for any positive, fixed iteration parameter; however, ϱ is quite close to one, and the convergence is not very rapid. Our problem is to choose a sequence of values for c_n that will materially reduce the number of iterations required to produce a satisfactory approximation to the solution of (8.1). This we shall do by specifying a variable set of parameters. Let

$$X_p(c) = \frac{4}{c(\Delta x)^2} \sin^2 \frac{\pi p \Delta x}{2}, \tag{8.7}$$

and let $\varrho_{pqr}(c)$ indicate the evaluation of ϱ_{pqr} corresponding to $X_p(c)$, $X_q(c)$, and $X_r(c)$ in (4.13). If

$$\alpha_n = \sum_{p,q,r=1}^{M-1} a_{pqr}^{(n)} \sin \pi p x \sin \pi q y \sin \pi r z, \tag{8.8}$$

then

$$\alpha_{n+1} = \sum_{p,q,r=1}^{M-1} a_{pqr}^{(0)} \cdot \prod_{k=0}^{n} \varrho_{pqr}(c_k) \cdot \sin \pi p x \sin \pi q y \sin \pi r z. \tag{8.9}$$

Thus, if we denote the operator that maps α_0 into α_{n+1} by A_n; i.e.,

$$\alpha_{n+1} = A_n \alpha_0, \tag{8.10}$$

then it is clear that the L_2 norm of A_n is given by

$$\|A_n\| = \max_{p,q,r} \left| \prod_{k=0}^{n} \varrho_{pqr}(c_k) \right|. \tag{8.11}$$

If the number n of iterations needed to complete the problem were known in advance, then the determination of an optimum sequence of iteration parameters would reduce to a minimax problem of some difficulty. It is clear that the k-th parameter will vary with n; thus, a complete treatment of the finding of optimum parameters would lead to a sequence of minimax problems. A colleague of the author has recently undertaken this effort; in the meantime, we shall have to settle for a cruder analysis.

In analyzing the applications of the earlier alternating direction methods to elliptic problems, the author has employed a finite geometric sequence to generate a parameter cycle. Let us again investigate such a choice. Note first that $\varrho_{pqr}(c)$ may be written in the form

$$\varrho_{pqr}(c) = 1 - \frac{2[X_p(c) + X_q(c) + X_r(c)]}{[1+X_p(c)][1+X_q(c)][1+X_r(c)]}. \tag{8.12}$$

The derivation of a geometric parameter sequence is facilitated by the following lemma.

Lemma 3. Let

$$\varrho = \varrho(a,b,c) = 1 - \frac{2(a+b+c)}{(1+a)(1+b)(1+c)}. \tag{8.13}$$

Then, if $\mu < 1 < \nu$,

$$\hat{\varrho}(\mu,\nu) = \max_{\substack{\mu \leqq a \leqq \nu \\ 0 \leqq b,c \leqq \nu}} |\varrho(a,b,c)| = \max\left[1 - \frac{6\nu}{(1+\nu)^3},\ 1 - \frac{2\mu}{1+\mu}\right]. \tag{8.14}$$

Proof. As

$$\frac{\partial \varrho}{\partial a} = 2(1+a)^{-2}(1+b)^{-1}(1+c)^{-1}(b+c-1);$$

$$\frac{\partial \varrho}{\partial a} \text{ is } \begin{cases} \text{nonnegative}, & b+c \geqq 1, \\ \text{nonpositive}, & b+c \leqq 1. \end{cases} \tag{8.15}$$

Similar relations hold by symmetry for $\frac{\partial \varrho}{\partial b}$ and $\frac{\partial \varrho}{\partial c}$. Let us consider maximizing $|\varrho|$ as a function of b and c for a fixed choice of a.

Case 1: $\mu \leqq a \leqq 1$.

If $\mu \leqq a \leqq 1$, then $\varrho(a, b, c)$, as a functoin of b and c on the square $0 \leqq b,\ c \leqq \nu$, has a saddle point at $b = c = 1 - a$. It is easy to see that

$$\begin{aligned} &\max_{0 \leqq b,\, c \leqq \nu} \varrho(a, b, c) = \max[\varrho(a, \nu, \nu), \varrho(a, 0, 0)], \\ &\min_{0 \leqq b,\, c \leqq \nu} \varrho(a, b, c) = \varrho(a, 0, \nu) = \varrho(a, \nu, 0), \qquad \mu \leqq a \leqq 1. \end{aligned} \tag{8.16}$$

By (8.15),

$$\begin{aligned} \max_{\substack{\mu \leqq a \leqq 1 \\ 0 \leqq b,\, c \leqq \nu}} \varrho(a, b, c) &= \max[\varrho(1, \nu, \nu), \varrho(\mu, 0, 0)] \\ &= \max\left[\frac{\nu^2}{(1+\nu)^2},\ 1 - \frac{2\mu}{1+\mu}\right], \end{aligned} \tag{8.17}$$

$$\begin{aligned} \min_{\substack{\mu \leqq a \leqq 1 \\ 0 \leqq b,\, c \leqq \nu}} \varrho(a, b, c) &= \varrho(\mu, \nu, 0) \\ &= \frac{(1-\mu)(1-\nu)}{(1+\mu)(1+\nu)}. \end{aligned} \tag{8.18}$$

Case 2: $1 \leqq a \leqq \nu$.

In this case it is easy to see that

$$\begin{aligned} &\max_{0 \leqq b,\, c \leqq \nu} \varrho(a, b, c) = \varrho(a, \nu, \nu), \\ &\min_{0 \leqq b,\, c \leqq \nu} \varrho(a, b, c) = \varrho(a, 0, 0), \qquad 1 \leqq a \leqq \nu. \end{aligned} \tag{8.19}$$

Again by (8.15),

$$\max_{\substack{1 \leqq a \leqq \nu \\ 0 \leqq b,\, c \leqq \nu}} \varrho(a, b, c) = \varrho(\nu, \nu, \nu) = 1 - \frac{6\nu}{(1+\nu)^3}, \tag{8.20}$$

$$\min_{\substack{1 \leqq a \leqq \nu \\ 0 \leqq b,\, c \leqq \nu}} \varrho(a, b, c) = \varrho(\nu, 0, 0) = 1 - \frac{2\nu}{1+\nu}. \tag{8.21}$$

Thus,

$$\begin{aligned} &\max_{\substack{\mu \leqq a \leqq \nu \\ 0 \leqq b,\, c \leqq \nu}} |\varrho(a, b, c)| \\ &\qquad = \max[\varrho(1, \nu, \nu), \varrho(\mu, 0, 0), -\varrho(\mu, \nu, 0), \varrho(\nu, \nu, \nu), -\varrho(\nu, 0, 0)]. \end{aligned} \tag{8.22}$$

By (8.15), $\varrho(\nu, \nu, \nu) > \varrho(1, \nu, \nu)$ and $-\varrho(\nu, 0, 0) > -\varrho(\mu, \nu, 0)$. A simple calculation shows $\varrho(\nu, \nu, \nu) > -\varrho(\nu, 0, 0)$ for $\nu \geqq 1$. Thus,

$$\max_{\substack{\mu \leqq a \leqq \nu \\ 0 \leqq b,\, c \leqq \nu}} |\varrho(a, b, c)| = \max[\varrho(\nu, \nu, \nu), \varrho(\mu, 0, 0)], \tag{8.23}$$

and the lemma is denonstrated.

We have proved a bit more than was stated; by symmetry we have

$$\begin{aligned} \hat{\varrho}(\mu, \nu) = \max\{|\varrho(a, b, c)| : &[\mu \leqq a \leqq \nu;\ 0 \leqq b,\ c \leqq \nu] \text{ or } \\ &[\mu \leqq b \leqq \nu;\ 0 \leqq a,\ c \leqq \nu] \text{ or } [\mu \leqq c \leqq \nu;\ 0 \leqq a,\ b \leqq \nu]\}. \end{aligned} \tag{8.24}$$

In our application of the above lemma, it will be advantageous to have the two terms giving the maximum of $|\varrho|$ equal.

Lemma 4. If $\nu \geqq 1$ and

$$\mu = \frac{3\nu(1+\nu)^{-3}}{1-3\nu(1+\nu)^{-3}} = \frac{3\nu}{1+3\nu^2+\nu^3}, \tag{8.25}$$

then

$$\hat{\varrho}(\mu,\nu) = 1 - \frac{6\nu}{(1+\nu)^3} = 1 - \frac{2\mu}{1+\mu}. \tag{8.26}$$

We are now in a position to choose a reasonably good parameter sequence $\{c_n\}$. Let

$$\zeta = \frac{4}{c(\Delta x)^2}, \qquad \xi_p = \sin^2 \frac{\pi p \Delta x}{2}. \tag{8.27}$$

Then,

$$\varrho_{pqr}(c) = 1 - \frac{2(\zeta\xi_p + \zeta\xi_q + \zeta\xi_r)}{(1+\zeta\xi_p)(1+\zeta\xi_q)(1+\zeta\xi_r)}. \tag{8.28}$$

Now, let us choose a sequence $\{\zeta_n\}$, $n=1, \ldots, P$, such that

$$\mu \leqq \zeta_n \xi_p \leqq \nu \tag{8.29}$$

for at least one n for every p, $p=1, \ldots, N-1$. As

$$\xi_1 = \sin^2 \frac{\pi \Delta x}{2}, \qquad \xi_{N-1} = \sin^2 \frac{\pi(N-1)\Delta x}{2} \approx 1, \tag{8.30}$$

it is sufficient to choose $\{\zeta_n\}$ such that there is at least one ζ_n for which

$$\mu \leqq \zeta_n \xi \leqq \nu \tag{8.31}$$

for every ξ such that

$$\sin^2 \frac{\pi \Delta x}{2} \leqq \xi \leqq 1. \tag{8.32}$$

To do this, set

$$\xi^{(1)} = \sin^2 \frac{\pi \Delta x}{2}, \tag{8.33}$$

and determine $\{\zeta_n, \xi^{(n+1)}\}$ by

$$\begin{aligned} \zeta_n \xi^{(n)} &= \mu, \\ \zeta_n \xi^{(n+1)} &= \nu. \end{aligned} \tag{8.34}$$

Then

$$\begin{aligned} \zeta_n &= \mu \left(\frac{\mu}{\nu}\right)^{n-1} \sin^{-2} \frac{\pi \Delta x}{2}, \\ \xi^{(n)} &= \left(\frac{\nu}{\mu}\right)^{n-1} \sin^{-2} \frac{\pi \Delta x}{2}. \end{aligned} \tag{8.35}$$

Also,

$$\mu \leqq \zeta_n \xi \leqq \nu, \qquad \xi^{(n)} \leqq \xi \leqq \xi^{(n+1)}. \tag{8.36}$$

We stop the sequence when $\xi^{(n)}$ crosses one:

$$\xi^{(P)} \approx 1, \tag{8.37}$$

or

$$P \sim \frac{2 \log csc\, \pi \Delta x/2}{\log \nu/\mu}. \tag{8.38}$$

By lemmas 3 and 4, if we iterate P times with the parameter sequence

$$c_n = \frac{4}{\zeta_n (\Delta x)^2} = \frac{4}{\mu}\left(\frac{\nu}{\mu}\right)^{n-1} \frac{\sin^2 \frac{\pi \Delta x}{2}}{(\Delta x)^2} \sim \frac{\pi^2}{\mu}\left(\frac{\nu}{\mu}\right)^{n-1}, \qquad n = 1, \ldots, P, \tag{8.39}$$

then

$$\|A_P\| \leqq \hat{\varrho}(\mu, \nu). \tag{8.40}$$

Thus, if we let

$$c_{Pm+n} = c_n, \qquad n = 1, \ldots, P, \qquad m = 0, 1, \ldots, \tag{8.41}$$

then

$$\|A_{Pm}\| \leqq \hat{\varrho}(\mu, \nu)^m, \qquad m = 1, 2, \ldots. \tag{8.42}$$

Now, let us determine the amount of calculation required to reduce $\|A_{Pm}\|$ below a preassigned $\varepsilon > 0$. If

$$\hat{\varrho}(\mu, \nu)^m \approx \varepsilon,$$

$$m \sim \frac{\log \varepsilon}{\log \hat{\varrho}(\mu, \nu)}, \quad \text{as} \quad \varepsilon \to 0. \tag{8.43}$$

Thus, the number of iterations required is

$$Pm \sim \frac{2 \log \varepsilon \log csc\, \pi\, \Delta x/2}{\log \hat{\varrho}(\mu, \nu) \log \nu/\mu}. \tag{8.44}$$

As the number of calculations per iteration is essentially a multiple K of $(\Delta x)^{-3}$, the total number of calculations needed to reduce $\|A_{Pm}\|$ below ε is

$$C \sim \frac{2K \log \varepsilon \log csc\, \pi\, \Delta x/2}{(\Delta x)^3 \log \hat{\varrho}(\mu, \nu) \log \nu/\mu}. \tag{8.45}$$

Assume that μ satisfies (8.25). Then, evaluating

$$\log \frac{1}{\hat{\varrho}(\mu, \nu)} \log \frac{\nu}{\mu} \tag{8.46}$$

for $\nu = 1(.01)2$ leads to the choice

$$\begin{aligned} &\nu_{\text{opt}} = 1.78, \\ &\mu_{\text{opt}} = 0{,}32, \\ &c_n = 12.5\,(0.556)^{n-1} \frac{\sin^2 \frac{\pi \Delta x}{2}}{(\Delta x)^2} \sim 30.8\,(0.556)^{n-1}, \end{aligned} \tag{8.47}$$

in order to maximize (8.46). If these choices are used, $\log \hat{\varrho}(\mu, \nu)^{-1} \log \nu/\mu = 1.16$.

Theorem 6. If μ is defined by (8.25) and $\{c_n\}$ by (8.39), the calculation required to reduce $\|A_{Pm}\|$ below ε is

$$O\left((\Delta x)^{-3} \log (\Delta x)^{-1}\right),$$

and, if $\{c_n\}$ is given by the particular choice (8.47), the total calculation C has the asymptotic bound

$$1.73\, K (\log \varepsilon^{-1})\, (\Delta x)^{-3} \log csc\, \pi\, \Delta x/2, \qquad \Delta x \to 0, \tag{8.48}$$

where K is the number of arithmetic operations per grid point required to perform one iteration.

The method of [*10*] leads to a relation of the form (8.48) with a multiplier of 4.1, rather than 1.73. As the value of K is exactly five larger for the new method than for that of [*10*], the use of (8.2) leads to a reduction of slightly more than one half in the calculation needed to approximate the solution of (8.1) by an alternating direction iteration procedure. Since successive over-relaxation requires $O\left((\Delta x)^{-4}\right)$ calculations to reduce the norm of the error as above, it is clear that (8.2) provides a more efficient iterative method for sufficiently small Δx.

9. Mildly Nonlinear Elliptic Equation, Direct Method

Consider the mildly nonlinear elliptic difference equation

$$(\Delta_x^2 + \Delta_y^2 + \Delta_z^2)\, w_{ijk} = \varphi(x_i, y_j, z_k, w_{ijk}) \tag{9.1}$$

on the unit cube. Apply the alternating direction iteration procedure (8.2) to (9.1) with φ being evaluated for each iteration:

$$\varphi = \varphi_n = \varphi(x_i, y_j, z_k, w_{i,j,k,n}). \tag{9.2}$$

Use the same parameter sequence $\{c_n\}$ as determined in the last section. We shall show that, if

$$\max\left|\frac{\partial \varphi}{\partial u}\right| = B \tag{9.3}$$

is sufficiently small, the iteration converges at a rate that maintains the $O\left((\Delta x)^{-3}\log(\Delta x)^{-1}\right)$ computing requirement for obtaining an approximate solution of (8.2). The bound B will tend to zero slowly as Δx tends to zero.

Again, let

$$\alpha_n = w - w_n \tag{9.4}$$

represent the difference between the solution w of the algebraic equations (9.1) and the n-th iterate w_n. Then, α_n satisfies the difference equation

$$\begin{aligned}(\Delta_x^2 + \Delta_y^2 + \Delta_z^2)(\alpha_{n+1} + \alpha_n) &= c_n(\alpha_{n+1} - \alpha_n) + c_n^{-1}(\Delta_x^2\Delta_y^2 + \Delta_y^2\Delta_z^2 + \Delta_z^2\Delta_x^2) \times \\ &\quad \times (\alpha_{n+1} - \alpha_n) - c_n^{-2}\Delta_x^2\Delta_y^2\Delta_z^2(\alpha_{n+1} - \alpha_n) + 2\beta_n\alpha_n,\end{aligned} \tag{9.5}$$

where β_{ijkn} denotes the partial derivative of φ with respect to u, evaluated to a point between (x_i, y_z, z_k, w_{ijk}) and $(x_i, y_j, z_k, w_{ijkn})$ as required by the mean value theorem. Expand α_n and $\beta_n\alpha_n$ into Fourier series:

$$\begin{aligned}\alpha_n &= \sum_{p,q,r=1}^{M-1} a_{pqr}^{(n)} \sin\pi p\, x \sin\pi q\, y \sin\pi r\, z,\\ \beta_n\alpha_n &= \sum_{p,q,r=1}^{M-1} b_{pqr}^{(n)} \sin\pi p\, x \sin\pi q\, y \sin\pi r\, z.\end{aligned} \tag{9.6}$$

By (4.12),

$$a_{pqr}^{(n+1)} = \varrho_{pqr}^{(n)} a_{pqr}^{(n)} + v_{pqr}^{(n)} b_{pqr}^{(n)} \Delta t_n, \qquad \Delta t_n = 2c_n^{-1}. \tag{9.7}$$

Lemma 5. For $n \geqq 0$,

$$a_{pqr}^{(n+1)} = a_{pqr}^{(0)} \prod_{k=0}^{n} \varrho_{pqr}^{(k)} + \sum_{k=0}^{n} v_{pqr}^{(k)} \Delta t_k\, b_{pqr}^{(k)} \prod_{j=k+1}^{n} \varrho_{pqr}^{(j)}, \tag{9.8}$$

interpreting

$$\prod_{j=n+1}^{n} \varrho_{pqr}^{(j)}$$

as one.

Proof. The argument is a straight-forward induction.

Lemma 6. For any choice of Δt,

$$|v_{pqr}\Delta t| \leqq \frac{2(\Delta x)^2}{27\sin^2\frac{\pi\Delta x}{2}} \sim \frac{8}{27\pi^2} \tag{9.9}$$

as Δx tends to zero.

Proof. For any choice of Δt, it is clear that

$$\begin{aligned}\max_{p,q,r}|v_{pqr}\Delta t| &= -v_{1,1,1}\Delta t\\ &= \frac{(\Delta x)^2}{\sin^2\frac{\pi\Delta x}{2}}\,\frac{\Delta t}{1+6\Delta t+12(\Delta t)^2+8(\Delta t)^3}.\end{aligned}$$

Thus,

$$\begin{aligned}|v_{pqr}\Delta t| &\leqq \frac{(\Delta x)^2}{\sin^2\frac{\pi\Delta x}{2}}\max_{s>0}\frac{s}{1+6s+12s^2+8s^3}\\ &= \frac{(\Delta x)^2}{\sin^2\frac{\pi\Delta x}{2}}\cdot\frac{2}{27},\end{aligned}$$

as the maximum of the function above occurs at $s=\frac{1}{4}$ and is $\frac{2}{27}$.

From (9.8) and the Parseval identity, it follows that

$$\begin{aligned}\|\alpha_{n+1}\|^2 &= \frac{1}{8}\sum_{p,q,r}(a_{pqr}^{(n+1)})^2\\ &= \frac{1}{8}\sum_{p,q,r}\left\{a_{pqr}^{(0)}\prod_{k=0}^{n}\varrho_{pqr}^{(k)}+\sum_{k=0}^{n}v_{pqr}^{(k)}\Delta t_k\, b_{pqr}^{(k)}\prod_{j=k+1}^{n}\varrho_{pqr}^{(j)}\right\}^2\\ &\leqq \frac{1+\delta^{-1}}{8}\sum_{p,q,r}(a_{pqr}^{(0)})^2\left(\prod_{k=0}^{n}\varrho_{pqr}^{(k)}\right)^2+\\ &\quad+\frac{1+\delta}{8}\sum_{p,q,r}\left[\sum_{k=0}^{n}v_{pqr}^{(k)}\Delta t_k\, b_{pqr}^{(k)}\prod_{j=k+1}^{n}\varrho_{pqr}^{(j)}\right]^2,\end{aligned} \tag{9.10}$$

where δ is an arbitrary positive number. For convenience set

$$\begin{aligned}L &= \frac{2(\Delta x)^2}{27\sin^2\frac{\pi\Delta x}{2}},\\ R_{kn} &= \max_{p,q,r}\left|\prod_{j=k}^{n}\varrho_{pqr}^{(j)}\right|.\end{aligned} \tag{9.11}$$

Then,

$$\|\alpha_{n+1}\|^2 \leqq (1+\delta^{-1})\,\|\alpha_0\|^2 R_{0,n}^2+\frac{1+\delta}{8}L^2\sum_{p,q,r}\left[\sum_{k=0}^{n}R_{k+1,n}\,b_{pqr}^{(k)}\right]^2. \tag{9.12}$$

Now,

$$\left[\sum_{k=0}^{n}R_{k+1,n}\,b_{pqr}^{(k)}\right]^2 \leqq \sum_{k=0}^{n}R_{k+1,n}\cdot\sum_{k=0}^{n}R_{k+1,n}(b_{pqr}^{(k)})^2, \tag{9.13}$$

and

$$\tfrac{1}{8}\sum_{p,q,r}\left[\sum_{k=0}^{n}R_{k+1,n}\,b_{pqr}^{(k)}\right]^2 \leqq \sum_{k=0}^{n}R_{k+1,n}\cdot\sum_{k=0}^{n}R_{k+1,n}\|\beta_k\alpha_k\|^2. \tag{9.14}$$

By (9.3),

$$\|\beta_n \alpha_n\| \leqq B \|\alpha_n\|; \tag{9.15}$$

therefore,

$$\|\alpha_{n+1}\|^2 \leqq (1+\delta^{-1}) \|\alpha_0\|^2 R_{0,n}^2 + (1+\delta) L^2 B^2 \Big(\sum_{k=0}^{n} R_{k+1,n}\Big) \sum_{k=0}^{n} R_{k+1\,n} \|\alpha_k\|^2. \tag{9.16}$$

The estimation of $\|\alpha_n\|$ can be facilitated by the following lemma.

Lemma 7. If

$$f_{n+1} = a\, e^{-\beta n} f_0 + b \sum_{k=0}^{n} e^{-\beta(n-k)} f_k, \qquad n \geqq 0, \tag{9.17}$$

then

$$f_{n+1} = (a+b)(b+e^{-\beta})^n f_0, \qquad n \geqq 0. \tag{9.18}$$

Proof. The proof is by induction. It is easily seen that (9.18) is satisfied for $n=0$; assume the relation to hold for f_k, $k \leqq n$. Then, a calculation involving interchanging the order of summation and expansion of $(b+e^{-\beta})^k$ by the binomial theorem shows that

$$f_{n+1} = (a+b) f_0 \sum_{j=1}^{n} b^j e^{-\beta(n-j)} \sum_{k=j}^{n} \binom{k-1}{j-1}.$$

As it can be shown by induction that

$$\sum_{k=j}^{n} \binom{k-1}{j-1} = \binom{n}{j}, \qquad j = 1, \ldots, n,$$

the relation (9.18) also holds for $n+1$.

In order to apply Lemma 7 to (9.16), it is necessary to estimate R_{kn}. If P again denotes the number of iterations per cycle of iteration, then

$$\begin{aligned} R_{kn} &\leqq \hat{\varrho}(\mu,\nu)^{\left[\frac{n-k}{P}\right]} \\ &\leqq \hat{\varrho}(\mu,\nu)^{\frac{n-k}{P}-1}. \end{aligned} \tag{9.19}$$

Consequently,

$$\sum_{k=0}^{n} R_{k+1\,n} < \hat{\varrho}(\mu,\nu)^{-1}\Big[1 - \hat{\varrho}(\mu,\nu)^{\frac{1}{P}}\Big]. \tag{9.20}$$

Let

$$e^{-\beta} = \hat{\varrho}(\mu,\nu)^{\frac{1}{P}}. \tag{9.21}$$

Weakening our inequality (9.16) slightly,

$$\begin{aligned} \|\alpha_{n+1}\|^2 \leqq{}& (1+\delta^{-1})\, \hat{\varrho}(\mu,\nu)^{-1} e^{-\beta n} \|\alpha_0\|^2 + \\ &+ (1+\delta) L^2 B^2 \hat{\varrho}(\mu,\nu)^{-2} (1-e^{-\beta})^{-1} \sum_{k=0}^{n} e^{-\beta(n-k)} \|\alpha_k\|^2. \end{aligned} \tag{9.22}$$

If

$$\begin{aligned} a &= (1+\delta^{-1})\, \hat{\varrho}(\mu,\nu)^{-1}, \\ b &= (1+\delta) L^2 B^2 \hat{\varrho}(\mu,\nu)^{-2} (1-e^{-\beta})^{-1}, \end{aligned} \tag{9.23}$$

then

$$\|\alpha_{n+1}\|^2 \leqq (a+b)(b+e^{-\beta})^n \|\alpha_0\|^2. \tag{9.24}$$

Clearly, for convergence it is sufficient that

$$b < 1 - e^{-\beta}. \tag{9.25}$$

This is equivalent to

$$B < \frac{\hat{\varrho}(\mu, \nu)(1 - e^{-\beta})}{L}, \tag{9.26}$$

since δ may be chosen arbitrarily small. If we choose μ and ν by (8.47) and P by (8.38),

$$\begin{gathered} \hat{\varrho}(\mu, \nu) = \frac{17}{33} = 0.502, \\ P \sim 1.17 \log \frac{2}{\pi \Delta x}. \end{gathered} \tag{9.27}$$

Thus, as Δx tends to zero, the requirement on B is that

$$B < 1.74\pi^2 \left[1 - \left(\frac{17}{33} \right)^{\frac{1}{1.17 \log \frac{2}{\pi \Delta x}}} \right]. \tag{9.28}$$

In particular,

$$\begin{aligned} B &< 0.47\pi^2, & \Delta x &= 1/10, \\ B &< 0.27\pi^2, & \Delta x &= 1/50, \\ B &< 0.23\pi^2, & \Delta x &= 1/100. \end{aligned} \tag{9.29}$$

The above results can be summarized in the following theorem.

Theorem 7. The alternating direction iteration process defined for the Laplace difference equation (8.1) converges for the mildly nonlinear elliptic difference equation (9.1) provided (9.28) is satisfied and φ is reevaluated after each iteration. Moreover, the number of calculations required remains

$$O\left((\Delta x)^{-3} \log (\Delta x)^{-1}\right).$$

The bound (9.28) is stronger than necessary for the existence of a solution of (9.1). In fact,

$$B < 3\pi^2 \tag{9.30}$$

is sufficient (but not necessary) for existence. The analysis leading to (9.28) was rather crude, and the author feels confident that a much better bound could be obtained by a more refined argument. The primary value of the above proof is that it provides the first mathematical argument validating a direct use of an alternating direction iteration for a more general problem than (8.1) while still using the full parameter sequence that numerical experiments have shown to be desirable for obtaining rapid convergence.

10. Mildly Nonlinear Elliptic Equation, Indirect Method

The author [7] recently discussed an indirect method for using alternating direction iteration on the mildly nonlinear elliptic equation (9.1). The process consisted of a two level iteration, the outer iteration being a Picard type iteration and the inner iteration being an alternating direction iteration. Let the superscript m index the outer iteration. Then the outer iteration is of the form

$$(10.1)\qquad (\Delta_x^2+\Delta_y^2+\Delta_z^2)\, w_{ijk}^{(m+1)} - A\, w_{ijk}^{(m+1)} = \varphi(x_i, y_j, z_k, w_{ijk}^{(m)}) - A\, w_{ijk}^{(m)} + r_{ijk}^{(m)},$$

where A is a constant to be specified below and $r_{ijk}^{(m)}$ is the residual at the end of the inner iteration used to approximate the solution of the linear algebraic equations resulting from the deletion of the residual term. Since φ is not evaluated for the solution (9.1), it is unnecessary to solve the linear equations exactly; however, $\|r^{(m)}\|$ will be required to go to zero as m tends to infinity. The solution of (10.1) for each m (i.e., the inner iteration) is by the alternating direction process (8.2) modified as follows:

$$(10.2)\qquad \begin{aligned} (\Delta_x^2 - c_n - 2A)\, w_{n+1}^{(m+1)*} &= -(\Delta_x^2 + 2\Delta_y^2 + 2\Delta_z^2 + c_n - 2A)\, w_n^{(m+1)} + \\ &\quad + 2[\varphi(w^{(m)}) - A\, w^{(m)}], \\ (\Delta_y^2 - c_n - 2A)\, w_{n+1}^{(m+1)**} &= \Delta_y^2 w_n^{(m+1)} - (c_n + 2A)\, w_{n+1}^{(m+1)*}, \\ (\Delta_z^2 - c_n - 2A)\, w_{n+1}^{(m+1)} &= \Delta_z^2 w_n^{(m+1)} - (c_n + 2A)\, w_{n+1}^{(m+1)**}, \\ w_0^{(m+1)} &= w^{(m)}. \end{aligned}$$

The same parameter sequence $\{c_n\}$ can be employed as before.

Let

$$(10.3)\qquad b \leqq \frac{\partial\varphi}{\partial u} \leqq B.$$

Then the optimum choice for A is

$$(10.4)\qquad A = \tfrac{1}{2}(B+b),$$

and let the restriction to be imposed on $\|r^{(m)}\|$ be

$$(10.5)\qquad \|r^{(m)}\| \leqq \frac{A+2\pi^2}{1+\varrho}\,\varrho^{m+1},$$

where

$$(10.6)\qquad \varrho = \frac{B-b}{B+b+6\pi^2}.$$

The following theorem follows directly from the argument of [7].

Theorem 8. If $b > -3\pi^2$ (the negative of the least eigenvalue of the Laplace differential operator on R, the unit cube) and if (10.5) is satisfied, then the solution of the iteration process defined by (10.1) and (10.2) converges to the solution of (9.1); moreover, the number of calculations required to reduce the error in the solution by a factor ε remains

$$O\big((\Delta x)^{-3}\log(\Delta x)^{-1}\big).$$

Note that this result is considerably stronger than that obtained for the direct method. One reason for this is that the argument leading to Theorem 8 does not ignore algebraic signs.

11. A Transformation

The form (9.1) is somewhat more general than it appears on first glance. Consider the linear elliptic differential equation

$$\nabla \cdot \left(p(x,y,z)\nabla u\right) - q(x,y,z)\,u = 0, \qquad p > 0, \tag{11.1}$$

on a rectangular parallelepiped. Let

$$v = p^{\frac{1}{2}}\,u. \tag{11.2}$$

It is well known that this transformation reduces (11.1) to the form

$$\Delta v = q^*(x,y,z)\,v, \tag{11.3}$$

where

$$q^* = \frac{q}{p} + \frac{\Delta p^{\frac{1}{2}}}{p^{\frac{1}{2}}}. \tag{11.4}$$

If q^* satisfies the condition (10.8) or its analogue on a different rectangular parallelepiped, then the iterative technique of the last section can be applied with assurance to (11.3). In particular, if p is a convex function (or, more generally, a subharmonic function) and $q \geqq 0$, (10.8) is satisfied for q^*. Also, for fixed p there exists Q such that $q(x,y,z) \geqq Q$ implies that (10.8) holds for q^*; however, if this strong absorption condition is imposed, a simpler iteration technique frequently is just as efficient as alternating direction. The author is not acquainted with a good practical criterion on p and q to insure the satisfaction of (10.8) by q^*, although it is clear that one would be valuable.

12. Generalizations

Most physical problems leading to parabolic and elliptic differential equations give rise to more general equations and regions than the ones that have been discussed above. The object here is to outline the practical application of the technique to some such problems; numerical experience with previous alternating direction methods indicates that these applications should be successful, although no proofs have been constructed.

Consider as an example the parabolic equation

$$\nabla \cdot \left(a(x,y,z,t)\nabla u\right) = b(x,y,z,t)\,u_t. \tag{12.1}$$

The generalization of equations (3.1) and (3.2) is

$$\begin{aligned} &\Delta_x(a_{n+\frac{1}{2}}\Delta_x w^*_{n+1}) - \frac{2b_{n+\frac{1}{2}}}{\Delta t} w^*_{n+1} \\ &= -\left[\Delta_x(a_{n+\frac{1}{2}}\Delta_x w_n) + 2\Delta_y(a_{n+\frac{1}{2}}\Delta_y w_n) + 2\Delta_z(a_{n+\frac{1}{2}}\Delta_z w_n) + \frac{2b_{n+\frac{1}{2}}}{\Delta t} w_n\right], \end{aligned} \tag{12.2a}$$

$$\Delta_y(a_{n+\frac{1}{2}}\Delta_y w^{**}_{n+1}) - \frac{2b_{n+\frac{1}{2}}}{\Delta t} w^{**}_{n+1} = \Delta_y(a_{n+\frac{1}{2}}\Delta_y w_n) - \frac{2b_{n+\frac{1}{2}}}{\Delta t} w^*_{n+1}, \tag{12.2b}$$

$$\Delta_z(a_{n+\frac{1}{2}}\Delta_z w_{n+1}) - \frac{2b_{n+\frac{1}{2}}}{\Delta t} w_{n+1} = \Delta_z(a_{n+\frac{1}{2}}\Delta_z w_n) - \frac{2b_{n+\frac{1}{2}}}{\Delta t} w^{**}_{n+1}, \tag{12.2c}$$

where

$$(12.3)\quad \Delta_x(a_{n+\frac{1}{2}}\Delta_x w_n) = \frac{a_{i+\frac{1}{2},j,k,n+\frac{1}{2}}(w_{i+1,j,k,n} - w_{ijkn}) - a_{i-\frac{1}{2},j,k,n+\frac{1}{2}}(w_{ijkn} - w_{i-1,j,k,n})}{(\Delta x)^2}$$

and $\Delta_y(a\Delta_y w)$ and $\Delta_z(a\Delta_z w)$ are defined similarly. The effective region for the difference equation can now be an arbitrary mesh domain; i.e., whenever ∂R is the union of portions of the planes $x=x_i$, $y=y_j$, or $z=z_k$. This equation is locally second order correct both in space and time; the author conjectures that it is also globally correct to the same order, unless the boundary conditions are not replaced to this accuracy.

If the coefficients also depend on u, the same type of prediction and correction that was applied to the mildly nonlinear parabolic equation earlier can be applied here. In similar fashions other parabolic equations can be treated.

Let us consider applying the alternating direction iteration directly to the elliptic difference equation

$$(12.4)\qquad \Delta_x(a\,\Delta_x w) + \Delta_y(a\,\Delta_y w) + \Delta_z(a\,\Delta_z w) = 0,$$

instead of trying the transformation (11.2). The iteration is similar to converting the elliptic problem to a parabolic problem of the form (12.1) with a and b independent of t. Now, the choice of $b(x, y, z)$ is entirely at the disposal of the user, and it is the experience of the author and his colleagues that this choice is quite significant. Obviously, the simplest choice is to take $b(x, y, z) \equiv 1$; however, if one looks at the induced parabolic problem physically, this is not realistic. The choice that has appeared to lead to the best results in several thousand applications of the older alternating direction iteration methods has been to use the local average of the coefficient $a(x, y, z)$:

$$(12.5)\quad b_{ijk} = \tfrac{1}{6}\left[a_{i+\frac{1}{2},j,k} + a_{i-\frac{1}{2},j,k} + a_{i,j+\frac{1}{2},k} + a_{i,j-\frac{1}{2},k} + a_{i,j,k+\frac{1}{2}} + a_{i,j,k-\frac{1}{2}}\right].$$

One motivation of this choice is that it tends to average the effect of the variable diffusivity over the entire region.

The choice of the parameter sequence $\{c_n\}$ is more delicate; the parameter c_n is to be interpreted as

$$(12.6)\qquad c_n = \frac{2}{\Delta t_n}$$

in (12.2). The following procedure has led to satisfactory iterative procedures for the older techniques. First, if $\hat{a}_{ijk}$ denotes any of the six values of a appearing in (12.5), let

$$(12.7)\qquad \begin{aligned} m_1 &= \min_{i,j,k} \frac{\hat{a}_{ijk}}{b_{ijk}}, \\ m_2 &= \max_{i,j,k} \frac{\hat{a}_{ijk}}{b_{ijk}}. \end{aligned}$$

Now, let Q be the smallest rectangular parallelepiped containing the region R. Consider the heat equation

$$(12.8)\qquad \Delta u = \frac{1}{\eta} u_t, \qquad (x, y, z) \in Q,$$

for all η such that $m_1 \leqq \eta \leqq m_2$. Then choose the parameter sequence $\{c_n\}$ such that the eigenvalues are covered for all such η; this has the effect of adding slightly to the number of parameters used in a cycle. The experience of PEACEMAN, RACHFORD, and the author with the older procedures for the choices of b_{ijk} and $\{c_n\}$ indicated here has been that the $O\left((\Delta x)^{-3} \log (\Delta x)^{-1}\right)$ computing estimate seems valid.

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