CENTRED DIFFERENCING AND THE BOX SCHEME FOR DIFFUSION - CONVECTION PROBLEMS

by

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ABSTRACT

Two discretizations of a constant coefficient diffusion-convection equation are compared. It is well known that to obtain acceptable results with centred differencing the spatial mesh size must be restricted in proportion to the strength of the convection. A similar restriction is shown to apply to the box scheme of H.B. Keller; however, a more quantitative examination of the two cases shows that the restriction is less severe for the box scheme. The errors in each are characterized by a false damping and phase shifting of solutions. It is shown that both effects are less prominent using the box scheme than using centred differences for problems with strong convection. The analysis is based on the observation that the box scheme can be viewed as having the same spatial discretization as the centred difference method, but with some spatial averaging of the temporal derivative. Such averaging features are commonly found in finite element methods also.

1. Introduction

The success of centred differences in handling problems with diffusion as the primary transport mechanism is well known to deteriorate severely when convection challenges or surpasses diffusion as the dominant transport mechanism of the model. Early studies of this were made by Peaceman and Rachford, [1], and Price, Varga, and Warren, [2]. More recently this phenomenon has received attention in a variety of contexts as the following selected references indicate: thermally driven flows [3], [4] steady viscous flows [5], [6], [7], flows in a porous medium [8], [9]. In these studies, the remedies sought for the degradation of performance in the centred difference analogs are variants of upwind differencing which adapt the scheme to the local transport conditions.

For one space dimensional problems, a method suggested by H. B. Keller ,[10], has been quite successful in a number of calculations of this type, particularly in fluid boundary layer problems ,(Keller and Cebeci [11] , Ackerberg and Phillips [12].) This approach is based on reducing the equations of the model to a first order system, and then using first differences to form a finite difference analog. For example, for the simple equation

$$(1.1) \qquad \partial u/\partial t = \partial^2 u/\partial x^2 + b(\partial u/\partial x)$$

we would introduce $w(x,t) = u(x,t)$, $z(x,t) = \partial u(x,t)/\partial x$ and write the equivalent first order system

(1.2) $$\partial w/\partial x = z$$

$$\partial z/\partial x = \partial w/\partial t - bz$$

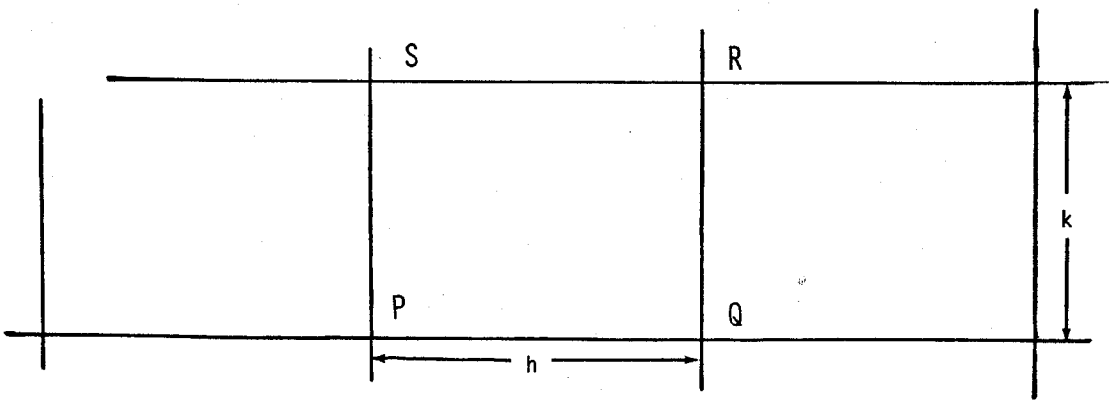

Figure 1

If we consider one rectangle, or 'box', shown in Figure 1, of a rectangular grid, we can write down the difference version of (1.2) as

(1.3)a $$(w(R) - w(S))/h = .5(z(R) + z(S))$$

(1.3)b $$.5\{(z(R) + z(Q)) - (z(S) + z(P))\}/h = .5\{(w(R) + w(S)) - (w(Q) + w(T))\}/k - b\{z(R) + z(S) + z(P) + z(Q)\}/4 .$$

The difference equations use first order differences and averages so as to obtain a second order accurate scheme while only coupling unknowns at the corners of one mesh 'box'. This method has been called the box scheme, and a hint at its effectiveness for problems of mixed transport type might be gained from the fact that it was discussed in an early paper on the mixed initial boundary value problem for hyperbolic systems by Thomee, [13].

In this paper, we attempt to indicate why the box scheme may be superior to centred difference methods for problems in which diffusion is not the dominant transport mechanism. To do this, we shall study the simple model equation (1.1) for a constant nonnegative parameter, b, and impose boundary conditions

$$u(0,t) = 0 \quad ; \quad u(1,t) = 0 \tag{1.4}$$

on the solution. A significant part of the problem of designing a satisfactory numerical method appears to be that of determining a suitable spatial discretization. Hence we shall retain the time variable as continuous but study two spatial discretizations to the uniformly spaced set of lines;

$$x = ih = x_i \quad ; \quad t > 0$$

$$i = 0, 1, \ldots, N \; ; \quad h = 1/N \; .$$

The semidiscrete problems corresponding to centred differencing and the box scheme will be systems of N-1 linear ordinary differential equations. Our comparison of these schemes will be based on a study of the relation of the fundamental modes of the semidiscrete problems with those of the original problem (1.1) with boundary conditions (1.4), as the parameters b and h vary.

The transient response from any initial condition can be expressed as a superposition of these modes. Hence we expect to be able to draw some conclusions for general transient problems about the relation of solutions of the semidiscrete analogs to solutions of the original problem. Computations which illustrate some of the points of our comparison are discussed.

2. The Semidiscrete Problems

The centred difference approximation is based on replacing the spatial operator $L = \partial^2/\partial x^2 + b\partial/\partial x$ by centred differences. The subscript 'j' on a function such as $V_j(t)$ will indicate that it is to be considered the time history of that function on the line $x = x_j$ of the semidiscrete mesh; $V(t)$ will be the N-1 vector with components $V_1(t), V_2(t), \ldots, V_{N-1}(t)$. Then the centred difference semidiscrete problem can be written as the initial value problem

$$(2.1) \qquad dV(t)/dt = A\,V(t) \;;\; V_j(0) = u_0(x_j) \quad j=1,2,\ldots,N-1$$

where A is the $(N-1)\times(N-1)$ tridiagonal matrix with $-2/h^2$ for its diagonal entries super diagonal entries of $(1+\beta)/h^2$, and subdiagonal entries of $(1-\beta)/h^2$, for $\beta = bh/2$.

In its form (1.3), the box scheme is the time discretization of

$$(2.2) \qquad (W_j(t) - W_{j-1}(t))/h = .5(Z_j(t) + Z_{j-1}(t))$$

$$(Z_j(t) - Z_{j-1}(t))/h = .5(W'_j(t) + W'_{j-1}(t)) - .5\,b\,(Z_j(t) + Z_{j-1}(t))$$

If, for two adjacent boxes, we add the second of these equations together, and eliminate the resulting spatial averages of Z using the first equation, we shall get

$$2(W_{j+1}(t) + W_{j-1}(t) - 2\,W_j(t))/h^2 =$$

$$.5(W'_{j+1}(t) + 2\,W'_j(t) + W'_{j-1}(t)) - b(W_{j+1}(t) - W_{j-1}(t))/h$$

This can be written as the initial value problem

$$(2.3) \qquad C^{-1}dW(t)/dt = A\,W(t) \quad ; \quad W_j(0) = u_0(x_j), \qquad j = 1,2,\ldots N-1$$

with A as in (2.1) and C^{-1} being the tridiagonal matrix with 1/2 for its diagonal entries and super and sub diagonal entries of 1/4.

Hence for this problem, the box scheme can be viewed as being the centred difference scheme modified by a space averaging of the time derivative. A similar observation has been made by Ackerberg and Phillips in [12] and incorporated in their computational procedure. When Galerkin methods of spatial discretization are used, a similar averaging of the terms in the time derivatives occurs e.g. [16]. For finite element methods, the matrix corresponding to C^{-1} is termed the mass matrix (see [14].)

3. Modal analysis

The solutions of (1.1), (2.1) and (2.3) can all be written as linear combinations of fundamental modes characteristic of each problem. The mth mode of (1.1) restricted to the mesh points is

$$U^{(m)}(t) = U^{(m)} \exp(\gamma_m t) \qquad (3.1a)$$

where the spatial part $U^{(m)}$ is a vector with components $U_j^{(m)}$ and

$$U_j^{(m)} = \exp(-bx_j/2)\sin(m\,x_j), \qquad (3.1b)$$

and time constants

$$\gamma_m = -(m^2\pi^2 + b^2/4). \qquad (3.1c)$$

The modes (3.1) show that an increasingly pronounced boundary layer forms at x=0 (i.e. at the outflow boundary,)as b increases.

Similarly, from the eigenvalues and eigenvectors of A and CA, we can obtain a fundamental system of modes for (2.1) and (2.3). We shall use $\gamma_m(A)$ and $\gamma_m(CA)$ for the eigenvalues of A and CA respectively, and $V^{(m)}$ and $W^{(m)}$ for the corresponding eigenvectors. Then the modes,

$$V^{(m)}(t) = V^{(m)} \exp(\gamma_m(A)t) \tag{3.2}$$

$$W^{(m)}(t) = W^{(m)} \exp(\gamma_m(CA)t)\ , \tag{3.3}$$

are semidiscrete analogs of (3.1). Some standard techniques for determining the spectra of tridiagonal Toeplitz matrices given in the Appendix are used to obtain the following expressions, using $\phi_m = m\pi h, \beta = bh/2$,

$$\gamma_m(A) = -h^{-2}\{4\sin^2(\phi_m/2) + 2\cos\phi_m\,(1-(1-\beta^2)^{1/2})\}, \tag{3.4a}$$

$$\gamma_m(CA) = -h^{-2}\{4\tan^2(\phi_m/2) + 2\cos\phi_m\,(4-(16-4\beta^2\sin^2\phi_m)^{1/2})/\sin^2\phi_m\}. \tag{3.4b}$$

For the eigenvectors, we have

$$V_j^{(m)} = \{(1-\beta)/(1+\beta)\}^{j/2} \sin(m\pi x_j), \tag{3.5a}$$

$$W_j^{(m)} = \{(1-\beta-h^2\gamma_m(CA)/4)/(1+\beta-h^2\gamma_m(CA)/4)\}^{j/2} \sin(m\pi x_j). \tag{3.5b}$$

Obviously, the parameter $\beta = bh/2$ plays an important role in these expressions. Looking at the time constants for the centred difference scheme, we see that the $\gamma_m(A)$'s are real only if $|\beta|<1$, and they lie in the interval of length $4(1-\beta^2)^{1/2}/h^2$ centered on $-2/h^2$.

If $|\beta| < 1$, we can write (3.5a) as

$$V_j^{(m)} = \exp(-b(A)x_j/2)\sin(m\pi x_j), \tag{3.6}$$

where $b(A) = h^{-1} \ln\{(1+\beta)/(1-\beta)\}$ (3.7)

to show its correspondence with the spatial variation of $U_j^{(m)}$ in (3.1). If $|\beta| = 1$, $\gamma_m(A) = -2\ h^{-2}$; and if $|\beta| > 1$, $\gamma_m(A)$ becomes complex with with $\mathrm{Re}(\gamma_m(A)) = -2\ h^{-2}$ and $V_j^{(m)}$ become complex as well. The qualitative description of these properties of the centred difference scheme have been discussed by Price, Varga and Warren in [2]. They use the concept of oscillation matrices and their analysis extends to variable coefficient problems. It is apparent that if $\beta > 1$ the matrix A ceases to be an oscillation matrix. Some implications of this have been discussed in a recent note by Hirsh and Rudy, [5], who refer to 2β as the cell Reynolds number.

The variation of the time constants of the box scheme is different and more complex. The $\gamma_m(CA)$'s are real if $|\beta| \le 2$, and, if $|\beta|$ grows beyond 2, they turn complex, two at a time, starting with the pair closest to the index [N/2]. More precisely, for specific index k, if $\beta > 2/|\sin(k\pi h)|$ then $\gamma_k(CA)$ is complex, but if $|\beta| < 2/|\sin(k\pi h)|$ then $\gamma_k(CA)$ is real and negative.

Thus, $W_j^{(m)}$ is real for $|\beta|<2/|\sin(m\pi h)|$ and

$$W_j^{(m)} = \exp(-b_m(CA)x_j/2)\sin(m\pi x_j) \tag{3.8}$$

where

$$b_m(CA) = h^{-2} \ln\{(1+\beta-h^2\gamma_m(CA)/4)/(1-\beta-h^2\gamma_m(CA)/4)\} \tag{3.9}$$

as compared with (3.1b) and (3.6). That is, the lower modes, which decay more slowly in time and hence are the most important modes, may remain real for a wider range of $|\beta|$, even for $|\beta|$ beyond 2.

To summarize then, as β increases the qualitative similarity between the modes of the semidiscrete problems and those of the original problem breaks down. However, the breakdown for the centred difference scheme, which occurs at $\beta = 1$, occurs for all modes simultaneously. This is quite drastic compared to the graduated breakdown occuring for the box scheme

which starts when $\beta = 2$ but in which the (usually dominant) lowest order modes are the 'last to go'.

We can get a more quantitative comparison of these modes, when they are real, by expanding their parameters $\gamma_m(A)$, $\gamma_m(CA)$, $b(A)$, and $b_m(CA)$, in power series in β and h. The results are;

$$\gamma_m(A) = \gamma_m + (m^4 \pi^4/12)h^2 + (m^2 \pi^2/2 - b^2/16)\beta^2 + O(\beta^4+h^4), \tag{3.10a}$$

$$\gamma_m(CA) = \gamma_m - (m^4 \pi^4/6)h^2 + (m^2 \pi^2/2)\beta^2 + O(\beta^4+h^4). \tag{3.10b}$$

and

$$b(A) = b + b\beta^2/3 + O(\beta^4), \tag{3.11a}$$

$$b_m(CA) = b + b(\beta^2/12 - m^2 \pi^2 h^2/4) + O(h^4 + \beta^4). \tag{3.11b}$$

For the simple heat equation with b=0, (3.10) shows that the leading term of the expansions of the error $|\gamma_m(A) - \gamma_m|$ is half that of $|\gamma_m(CA) - \gamma_m|$. A more significant observation is that the leading terms (at least) of the expansion of the error in $\gamma_m(CA)$ in β and h are independent of b, while those of $\gamma_m(A)$ have coefficients proportional to b^2. Moreover, (3.11) shows that for larger $|b|$, the box scheme is better in approximating the mode shape constant, b, for a fixed h. These observations suggest that the centred difference scheme should be superior for b=0 or b small, but the box scheme should be better for larger b.

In figure 2, a graph is given showing the variation of errors with β. The variation of β from .2 to 1.2 by .05 was obtained by fixing h at .02 and varying b from 20 to 120 by 5. The four curves which appear represent the errors in the propagation of two different initial profiles by each of the two methods. The initial profiles are those of the first and third modes of (1.1) and the error is the relative error averaged over the leftmost third of the meshpoints at time $t=1/\gamma_1$ for the first mode and $t=1/\gamma_3$ for the third mode. Several similar measures of error were tried but no significant difference between them was noticed.

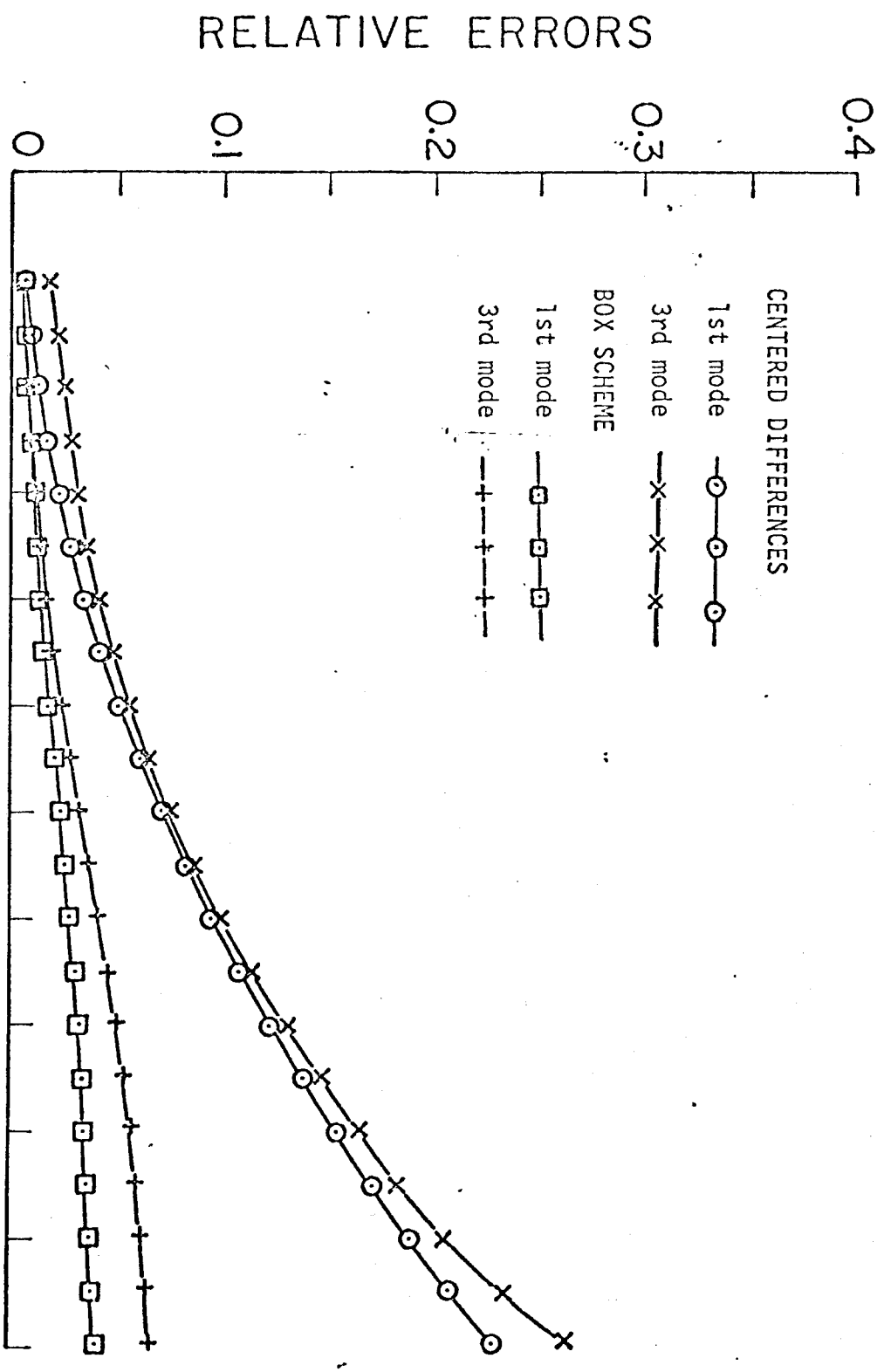

FIGURE 2: Variation of Relative Errors with Beta

4. Pseudo Modes

For the pure diffusion case, (b=0), the initial profiles of the modes for a fixed wave number are the same for all three problems. Simple computations show that the error in propagation of one of these profiles by the centred differences scheme is about half that of the box scheme, and has the opposite sign as predicted by (3.10).

However, for $b\neq 0$, the initial spatial profiles of the modes of the mth wave number do not coincide for any pair chosen from the original or the two semidiscrete problems. This complicates the designing of computations to demonstrate the features of the preceding modal analysis. We can, however, find quite simple analytic forms for certain solutions of the semidiscrete equations which have the same initial profile $\exp(-bx/2)\sin(m\pi x)$, as the mth mode of the continuous problem. These solutions do not satisfy the boundary conditions exactly. However, their values at x=0 and x=1 remain small for short times in a way made more precise by their expressions given below. Hence we may expect them to approximate the solutions of the semidiscrete problems with initial profile $\exp(-bx/2)\sin(m\pi x)$ at least away from the boundaries. These approximate solutions we shall call pseudo modes.

The mth pseudo mode for the semidiscretizations of the centred difference scheme, (2.1), and the box scheme, (2.3), we shall denote by $Vs^{(m)}(t)$ and $Ws^{(m)}(t)$ respectively.

$$Vs^{(m)} = \exp(-bx/2)\sin[m\pi x + I_m(A)t]\exp(R_m(A)t), \tag{4.1}$$

$$Ws^{(m)} = \exp(-bx/2)\sin[m\pi x + I_m(CA)t]\exp(R_m(CA)t). \tag{4.2}$$

The mode parameters $R_m(A)$ and $I_m(A)$ for the centred difference scheme are

$$R_m(A) = h^{-2}\{-2+\cos(\phi_m)[(\exp(\beta)+\exp(-\beta))-\beta(\exp(\beta)-\exp(-\beta))]\}$$

$$I_m(A)=h^{-2}\{\sin(\phi_m)[\beta(\exp(\beta)+\exp(-\beta))-(\exp(\beta)-\exp(-\beta))]\} \tag{4.3a}$$

and those for the box scheme are

$$R_m(CA) = \{R_m(A)p+I_m(A)q\}/(p^2+q^2) \tag{4.4c}$$

$$I_m(CA) = \{I_m(A)p-R_m(A)q\}/(p^2+q^2), \tag{4.4d}$$

$$p=1/2+\cos\phi_m[\exp(\beta)+\exp(-\beta)]/4, \tag{4.4e}$$

$$q=-\sin\phi_m[\exp(\beta)-\exp(-\beta)]/4. \tag{4.4f}$$

These parameters are determined by identifying them as the real and imaginary parts of a complex parameter $\alpha = R+iI$. Then α is determined, for the centred difference discretization by requiring $y(x,t)=\exp(-bx/2+im\pi x+\alpha t)$ to satisfy

$$dy(x,t)/dt=h^{-2}\{y(x+h,t)-2y(x,t)+y(x-h,t)\} +b\{y(x+h,t))-y(x-h,t)\}/(2h) \tag{4.5}$$

The equating of real and imaginary parts of both sides of (4.5) yields (4.3). For the box scheme, α is determined by requiring $y(x,t)$ to satisfy (4.5) with the left side replaced by

$$.25\ dy(x+h,t)/dt+.5\ dy(x,t)/dt+.25\ dy(x-h,t)/dt. \tag{4.6}$$

To see the connection between these solutions, and the modes of the original problem, we again expand the mode parameters R and I in power series in h and β to get

$$R_m(A) = \gamma_m+(m^4\pi^4/12)h + (m^2\pi^2/2-b^2/16)\beta^2 + 0(\beta^4+h^4), \tag{4.7a}$$

$$R_m(CA) = \gamma_m-(m^4\pi^4/6)h^2 + (m^2\pi^2/2)\beta^2 + 0(\beta^4+h^4). \tag{4.7b}$$

$$I_m(A)=m\pi[b\beta^2/3] + 0(\beta^4), \tag{4.8a}$$

$$I_m(CA)=m\pi[b(\beta^2/12 - m^2\pi^2h^2/4)] + 0(h^4 + \beta^4). \tag{4.8b}$$

It is interesting to note that the leading error terms in $R_m(A)$ and $R_m(CA)$ are exactly the same as the corresponding leading error terms in the time constants for the semidiscrete modes given in (3.10)(errors meaning deviations from the time constants of the original problem)

The pseudo modes are intended to serve as models for predicting the propagation of the continuous modes' inital profiles by the semi-discretizations. Consider, for example, the leading error term in β^2 for $R_m(A)$. It predicts an erroneous damping if $m^2\pi^2/2<b^2/16$ which depends on b and which is most severe in the modes of smallest wave number. The corresponding term of the error in $R_m(CA)$ predicts an amplification of the modes which is uniform in b, and increases with the wave number. Similarly the terms $I_m(A)$ and $I_m(CA)$ represent erroneous phase shifts in the time evolution of the discretized solutions. The leading terms of these phase

shifts predicts that at least for the lower wave numbers the phase shift in the box scheme is less than a quarter of that for the centred difference scheme. However, as will be seen in Figures 5 through 8 (discussed below) these two time behaviour 'errors' compensate for each other so that the pseudo mode is substantially closer to the continuous problem's mode than the discrete problem's mode is, and the same is true of the approximate solution.

We shall examine a particular but representative case in more detail. We choose b=60. and h=.02, so that β=.60. In this case, the mode parameters for the first and third modes are:

i) for the exact modes
   b= 60., γ_1= -909.9, γ_3 = 989.0

ii) for the centred difference method modes
   b(A) = 69.32, γ_1(A)= -1007.9, γ_3(A)= -1070.9
   and for its pseudo modes
   R_1(A) = -990.6, R_3(A)= - 1053.8

iii) for the box scheme
   b_1(CA)= 61.84, b_3(CA)= 61.37
   γ_1(CA)= -908.2, γ_3= -974.1
   and for its pseudo modes
   R_1(CA)= -907.6, R_3(CA)= -974.3

The spatial profiles of these modes are shown in Figures 3 through 8. These profiles are taken for $t=1/\gamma_1$ for the first modes and $t=1/\gamma_3$ for the third modes. In each case twenty time steps were used to reach the final time from t=0. The figures show four graphs:

i) the mode of the exact problem (3.1) shown as a dashed line

ii) the pseudo mode for the method shown as a dashed-dotted line (4.1, 4.2)

iii) the mode of the (semidiscrete) method shown as a small cross at the spatial mesh points, (3.5)
   and

iv) the solution of the initial value problem (2.1, 2.3) by the method (initial values equal to those of i) and ii)) shown as large 'x' at the spatial mesh points.

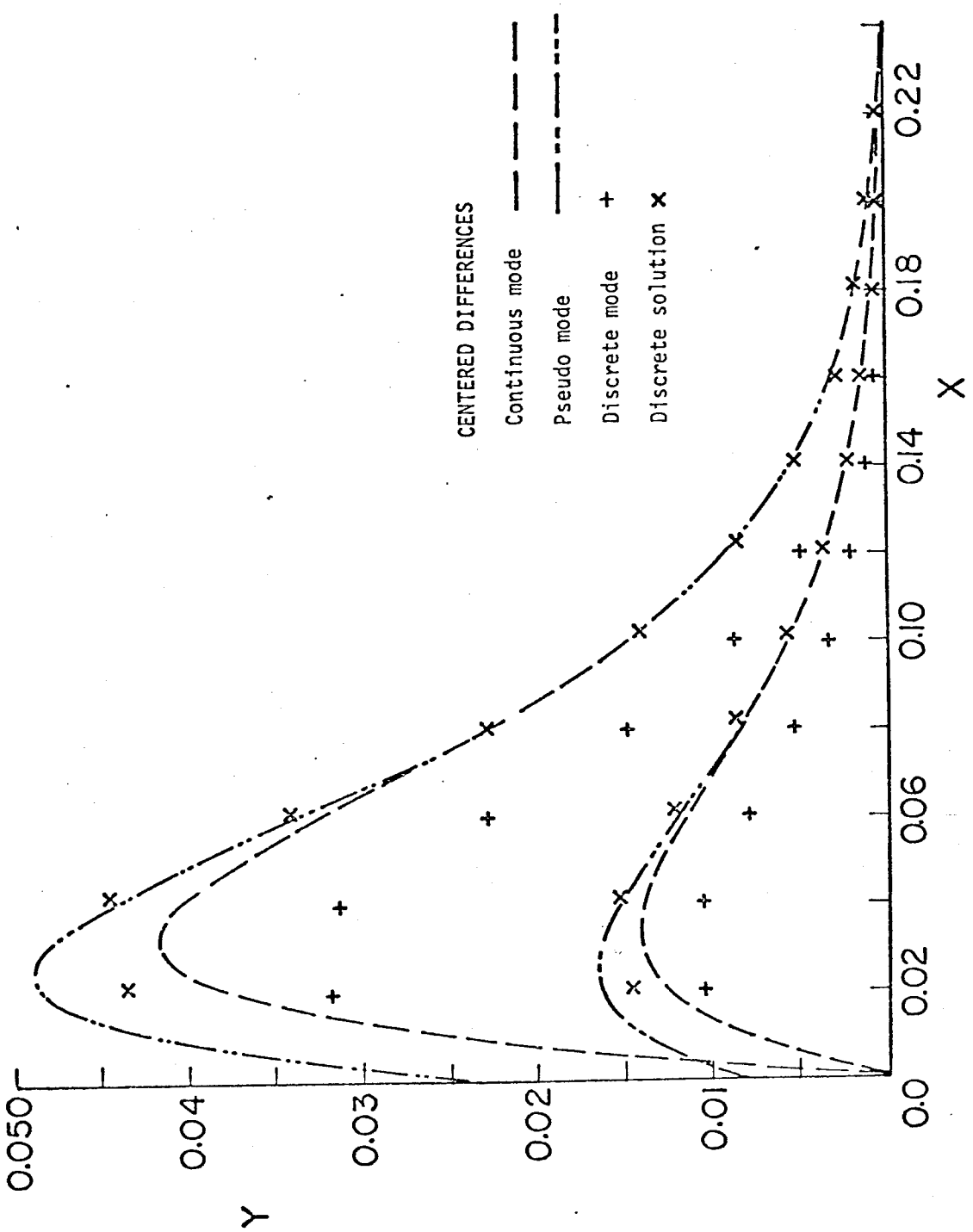

FIGURE 3: Profiles of Continuous and Centered Difference Modes

(lower curve - 1st mode upper curve - 3rd mode)

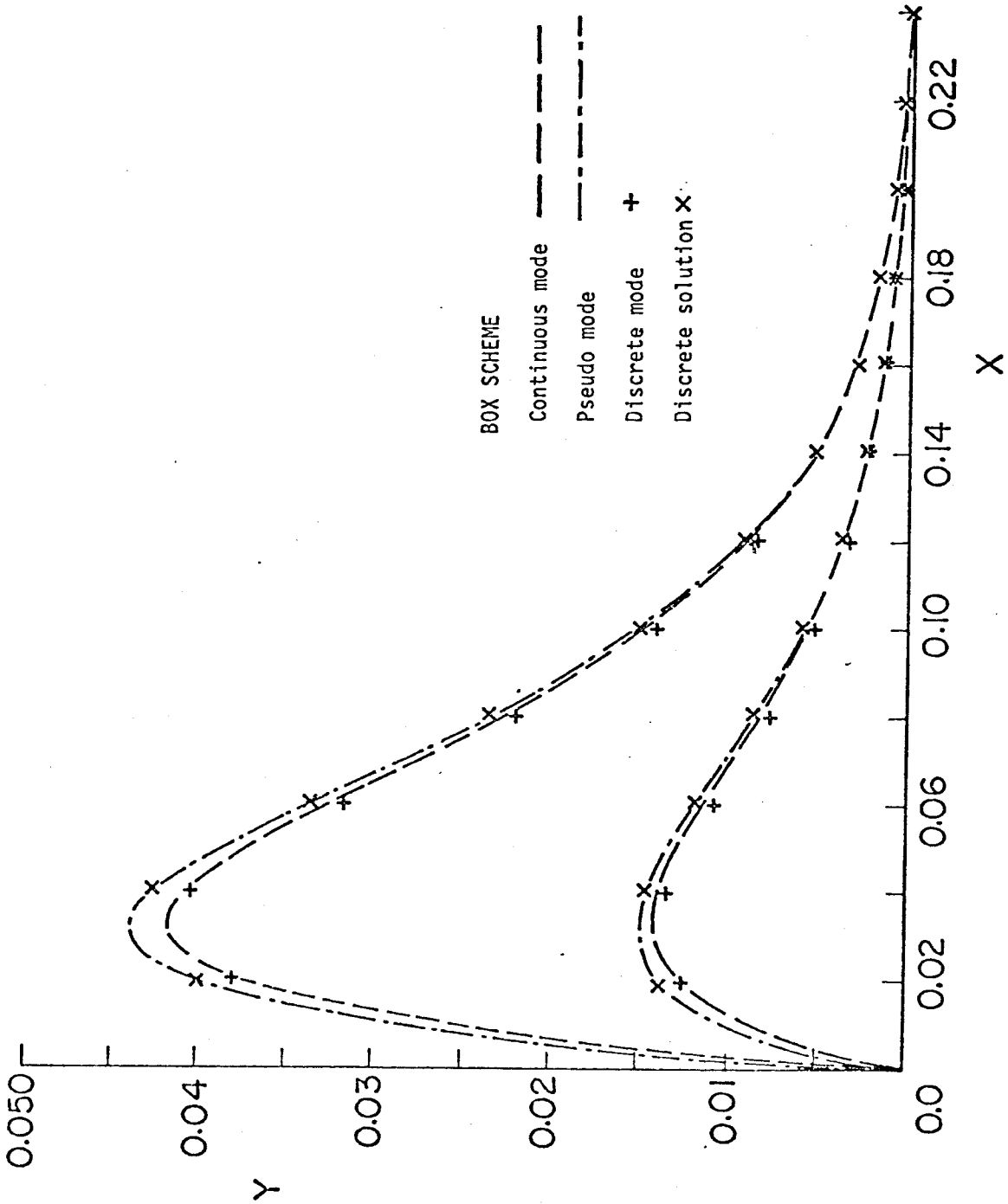

FIGURE 4: Profiles of Continuous and Box Scheme Modes
(lower curve - 1st mode; upper curve - 3rd mode)

There are several different points of comparison that can be made here. The pseudo modes, ii), are intended to be an analytical model for the computed solution, iv), of the initial value problem. This latter is, of course, the numerical approximation by the method to i). The comparison of the mode of the exact problem, i), to the corresponding mode of the semi-discrete problems, iii), indicates the degree of accuracy to which the continuous mode, i), can be approximated by the discrete mode, iii), of the method. If the discrete mode, iii), approximates poorly the continuous mode, i), we expect poor agreement between the numerical solution, iv), and the exact solution, i). Actually, Figure 3 shows that this indeed happens to the central differencing scheme. On the other hand, Figure 4 shows good agreement between both the discrete mode and the discrete solution to the continuous mode, in the case of the box scheme. In both Figs. 3 and 4, the pseudo modes predict the discrete solutions reasonably well, showing their capability as an analytical model for the discrete solution. In fact, the analytical forms (4.1) and (4.2) of the pseudo modes can further quantify the errors in terms of damping or amplifying, and phase-shifts in the numerical solution. To show this, we scale up each of the profiles i) - iv) by the factor $\exp(bx/2)$ and examine the resulting "expanded" profiles as shown in Figs. 5-8. As explained earlier, for a fixed time t, the damping error in $R_m(A)$, (centred differences,), is most severe in the modes of smallest wave number, whereas $R_m(CA)$ (box scheme), results in an amplification of the modes, which is uniform in b but increases with the wave number. Superimposed on these errors are the phase-shift errors due to $I_m(A)$ and $I_m(CA)$ in (4.1) and (4.2) which are most evident in Fig. 7, the third mode of the centred difference approach.

A major motivation for examining the modes of a problem is to be able to make 'educated guesses' about the behaviour of the more general initial value problems which are linear combinations of modes. In comparing our approximating semidiscrete problem to its continuous counterpart, the notion of 'corresponding mode' is fairly clear on a qualitative basis (e.g. number of interior zeros). But there is also some implication that if the restriction to the mesh lines of a general initial value problem were

$$u_i(t) = \sum_m a_m U_i^{(m)}(t) \tag{4.9}$$

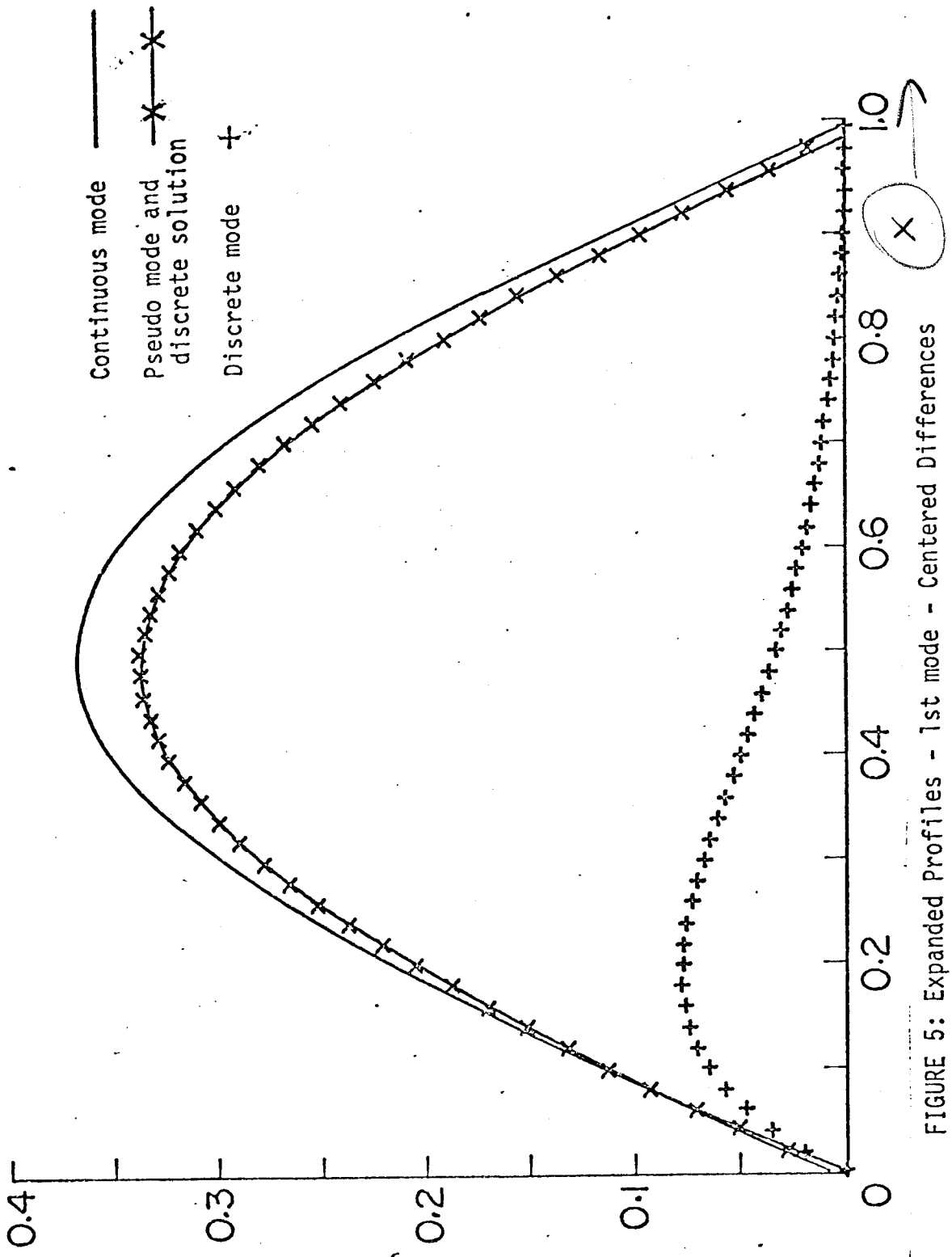

FIGURE 5: Expanded Profiles - 1st mode - Centered Differences

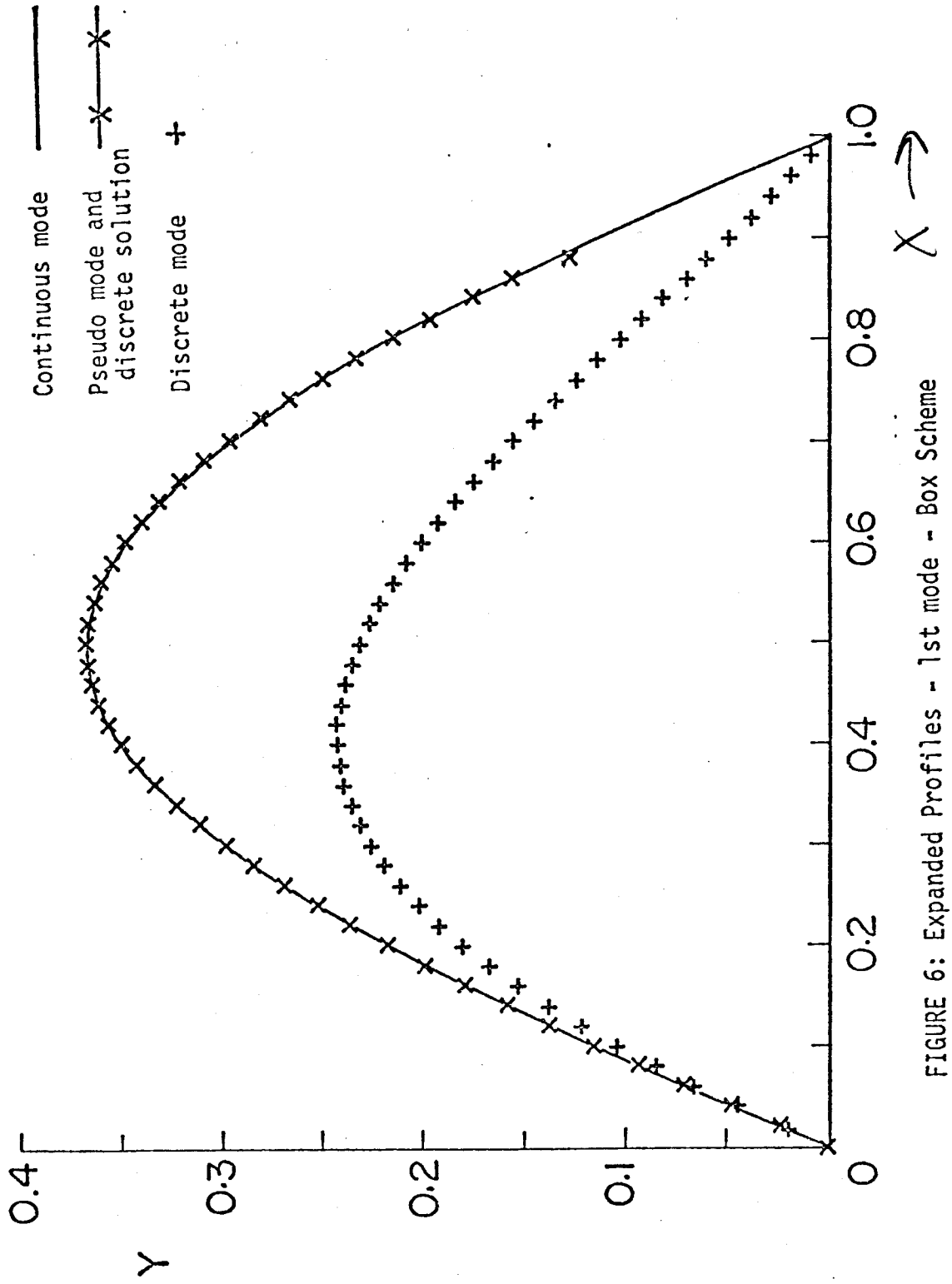

FIGURE 6: Expanded Profiles - 1st mode - Box Scheme

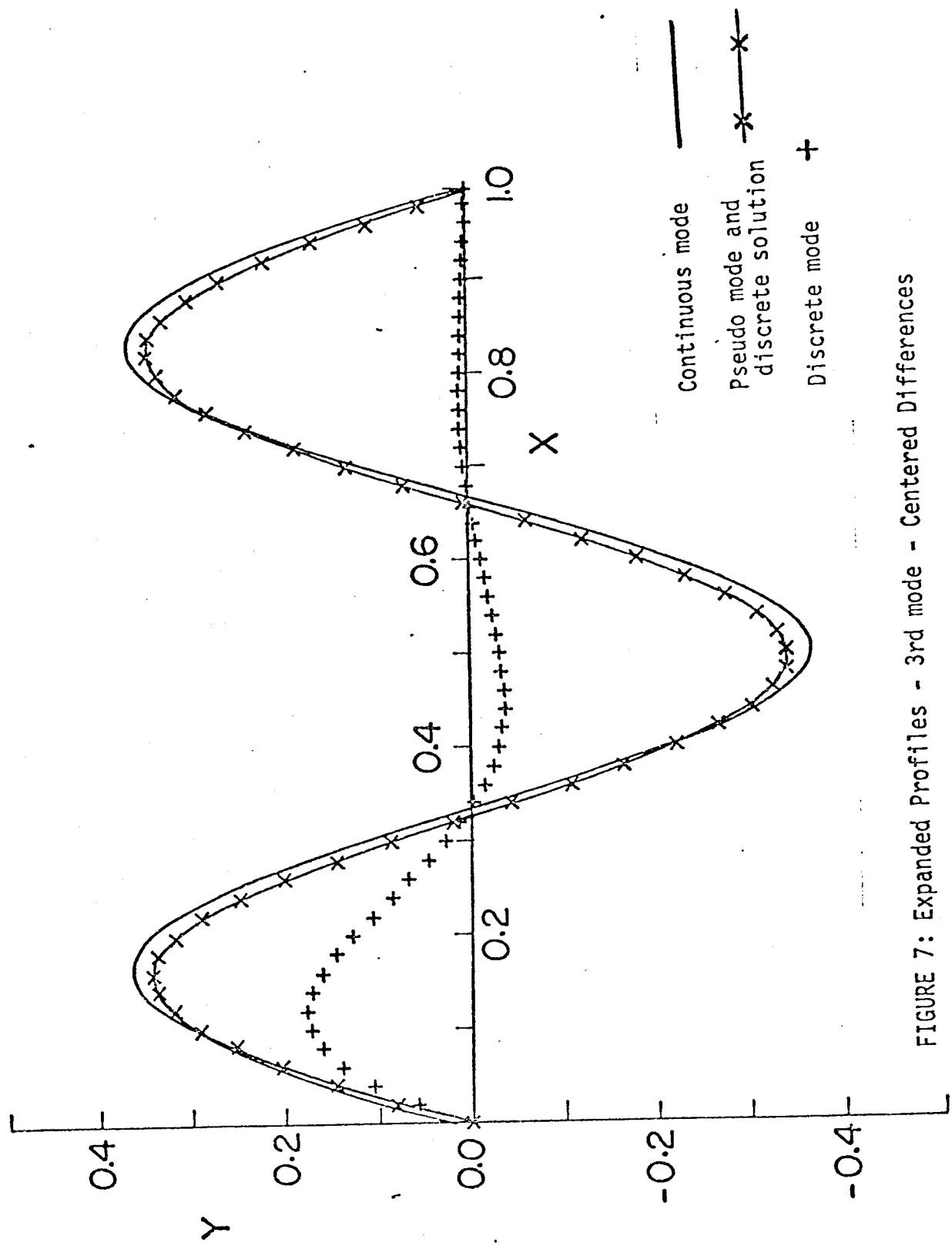

FIGURE 7: Expanded Profiles - 3rd mode - Centered Differences

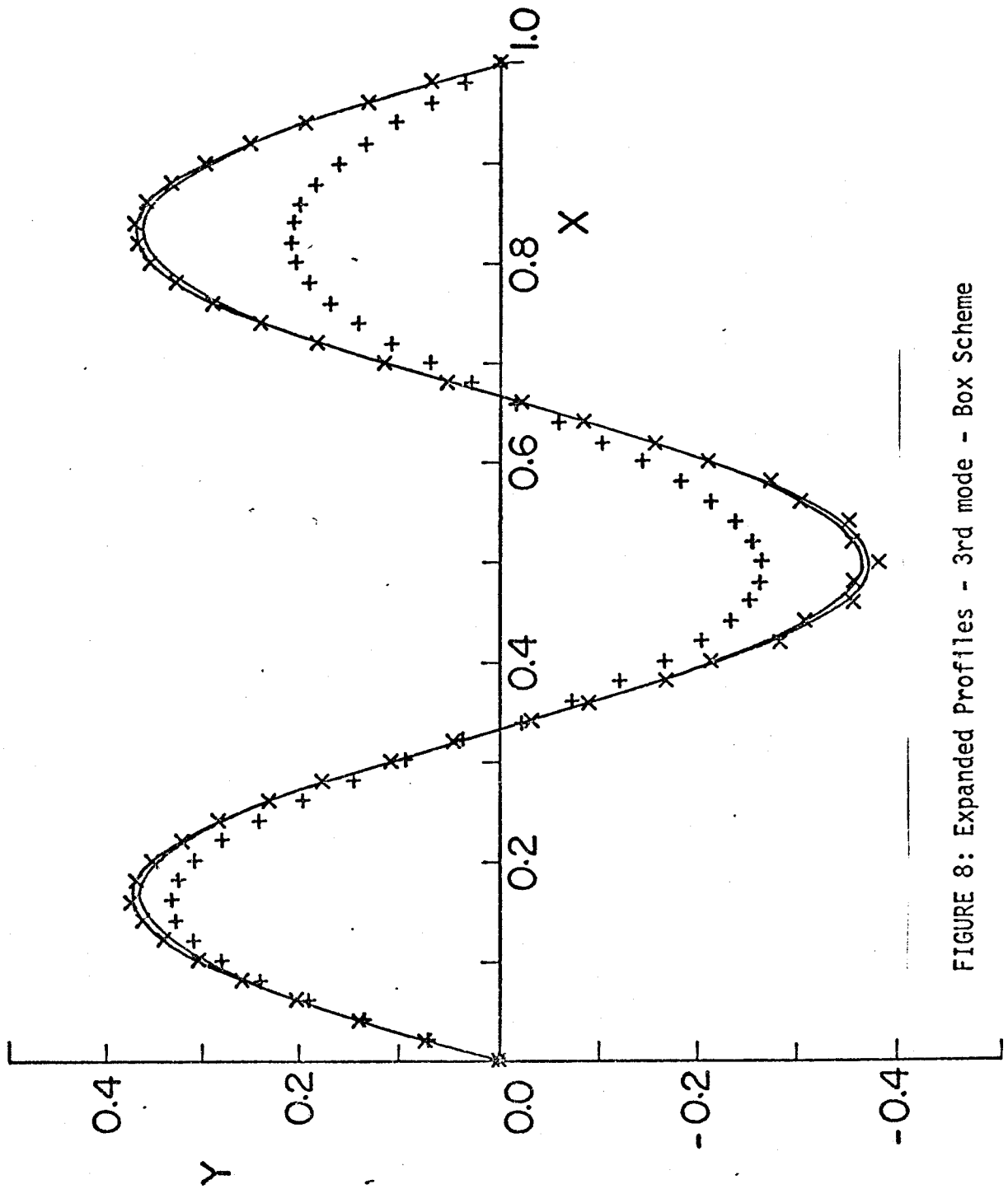

FIGURE 8: Expanded Profiles - 3rd mode - Box Scheme

then the semidiscrete approximation could be thought of, at least for intuitive guess purposes, as

$$v_i(t) = \sum_m a_m V_i^{(m)}(t) \tag{4.10}$$

or

$$w_i(t) = \sum_m a_m W_i^{(m)}(t) \tag{4.11}$$

The errors in the semidiscrete mode parameters, [primarily b(A) and $b_m(CA)$] indicate that the corresponding modes are, in fact, too dissimilar to provide much of a basis for the approximations in (4.10) or (4.11), at least for the range of mesh sizes yielding a few percent relative error. However, the correspondence between the propagation by the numerical method of the initial mode shape for the continuous problem and the method's pseudo mode seems quite close. Hence we feel that thinking in terms of expansions in pseudo modes

i.e.
$$vs_i(t) = \sum_m a_m Vs_i^{(m)}(t)$$

or
$$ws_i(t) = \sum_m a_m Ws_i^{(m)}(t)$$

provides a viable base for 'educated guessing'.

It appears on this basis that as the convective terms of a one dimensional transport model become more significant the box scheme enjoys an increasing accuracy advantage over centred differencing for the same mesh. It should be noted here that the box scheme has the more significant practical advantage of retaining second order accuracy on general non-uniform meshes. The qualitative behaviour of the time constants for the centred difference scheme with non-uniform meshes, i.e. becoming complex when $\beta > 1$, was established in [2]. (Here β varies with the position in the mesh.) The authors have been able to show that the time constants for the box scheme, for variable meshes, are real and negative if $\beta < 1$, (again, for local β); however we have been unable to establish this qualitative fact for the range $0 < \beta < 2$ as suggested by this analysis of the uniform mesh case.

Alternatively, these observations can be viewed as a beneficial effect resulting from a particular spatial averaging of the time derivatives of the semi-discretization. Similar averagings are done by the

'mass' matrix of variational semidiscretizations using basis functions of small support (e.g. [16],) and a discussion of these is made in [17].

BIBLIOGRAPHY

[1] Peaceman, D.W. and Rachford, H.H., "Numerical Calculation of Multi-dimensional Miscible Displacement", Soc. Petrol. Eng. J., vol.2 (1962), pp.327-338.

[2] Price, H.S., Varga, R.S. and Warren, J.E., "Application of Oscillation Matrices to Diffusion-Convection Equations", J. Math. and Physics, vol.45 (1966), pp.301-311.

[3] Denny, V.E. and Clever, R.M., "Comparisons of Galerkin and Finite Difference Methods for Solving Highly Nonlinear Thermally Driven Flows", J. Comp. Phys., vol.16 (1974), pp.271-284.

[4] Runchal, A.K., "Convergence and Accuracy of Three Finite Difference Schemes for a Two-dimensional Conduction and Convection Problem", Inter. J. for Num. Methods in Eng., vol.4 (1972),pp.541-550.

[5] Hirsh, R.S. and Rudy, D.H., "The Role of Diagonal Dominance and Cell Reynolds Number in Implicit Difference Methods for Fluid Mechanics Problems", J. Comp. Phys., vol.16 (1974), pp.304-310.

[6] Dorr, F.W., "An Example of Ill-Conditioning in the Numerical Solution of Singular Perturbation Problems", Math. of Comp., vol.25 (1971), pp. 271-283.

[7] Raithby, G.D., and Torrance, K.E., "Upstream-Weighted Differencing Schemes and Their Application to Elliptic Problems Involving Fluid Flow", Comp. and Fluids, vol.2 (1974), pp.191-206.

[8] Todd, M.R., O'dell, P.M., and Hirasaki, G.J., "Methods for Increased Accuracy in Numerical Reservoir Simulators", Soc. Petrol. Eng. J., vol.12 (1972), pp.515-530.

[9] Tagamets and Sternberg, "A Predictor-Corrector Method for Solving the Convection-Dispersion Equation for Adsorption in Porous Media", Water Resources Research, vol.10 (1974), pp.1003-1011.

[10] Keller, H.B., "A New Difference Scheme for Parabolic Problems", Numerical Solution of Partial Differential Equations II (SYNSPADE 1970), B. Hubbard ed. Academic Press.

[11] Keller, H.B. and Cebeci, T., "Accurate Numerical Methods for Boundary-Layer Flows - II. Two-dimensional Turbulent Flows", AIAA J., vol.10 (1972), pp.1193-1201.

[12] Ackerberg, R.C., and Phillips, J.H., "The unsteady laminar boundary layer on a semi-infinite flat plate due to small fluctuations in the magnitudes of the free stream velocity", J. Fluid Mech., vol.51 (1972), pp.137-157.

[13] Thomée, V., "A stable Difference Scheme for the Mixed Boundary Problem for a Hyperbolic First Order System in Two Dimensions", J. SIAM, vol. 10 (1962), pp. 229-245.

[14] Zlamal, M., "Finite Element Methods for Parabolic Equations", Conference on the Numerical Solution of Differential Equations, Proc. Lecture Notes in Mathematics, vol. 363, Springer-Verlag, 1974.

[15] Jordan, C., "Calculus of Finite Differences", Chelsea Publ. Co., N.Y., 1950.

[16] Price, H.S., Cavendish, J.C. and Varga, R.S., "Numerical Methods of Higher-Order Accuracy for Diffusion-Convection Equations", Soc. Petrol. Eng. J., 243(3), (1968), pp. 293-303.

[17] Gresho, P.M., Lee R.L., and Sani, R.L., "Advection Dominated Flows with Emphasis on the Consequences of Mass Lumping", presented at the Second International Symposium on Finite Element Methods in Flow Problems, to appear.

Appendix

We shall outline the proofs for the expressions in (3.4)-(3.5) and for the expansions in (3.10),(3.11),(4.7) and (4.8). We first derive the expression (3.4)-(3.5), using the following lemma on the eigenvalues and eigenvectors of a tridiagonal Toeplitz matrix :

Lemma A

Let L be an (N-1)x(N-1) tridiagonal Toeplitz matrix such that $L_{i,i-1} = l_1$, $i=2,\ldots,N-1$; $L_{i,i} = l_2$, $i=1,\ldots,N-1$; $L_{i,i+1} = l_3$, $i=1,\ldots,N-2$; $L_{i,j} = 0$, otherwise. Let γ_m be the mth eigenvalue of L and $Y^{(m)}$ be the corresponding eigenvector with components $Y^{(m)}_j$, $j=1,..,N-1$. Then,

$$\gamma_m = l_2 + 2(l_1 l_3)^{1/2} \cos \phi_m , \qquad (B.1)$$

$$Y^{(m)}_j = (l_1/l_3)^{j/2} \sin(j\phi_m) , j=1,..,N-1, \qquad (B.2)$$

where $\phi_m = m\pi/N$.

For a proof of this lemma, we refer the reader to [15].

Now,(3.4) follows immediately. For the box scheme, we observe that the eigenvalue problem,

$$CA\, W^{(m)} = \gamma_m (CA)\, W^{(m)} , \qquad (B.3)$$

is identical with the generalized eigenvalue problem,

$$A\, W^{(m)} = \gamma_m (CA)\, C^{-1} W^{(m)} , \qquad (B.4)$$

or, we can consider the problem

$$(A - \gamma_m (CA) C^{-1}) W_j^{(m)} = \alpha_m W_j^{(m)}, \qquad (B.5)$$

and ask for $\alpha_m = 0$, $m=1,..,N-1$. Using Lemma A, and after discarding of some extraneous roots in the equations $\alpha_m = 0$, we obtain (3.5).