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EVALUATION OF LEAST SQUARES TIME STEPPING PROCEDURES FOR TRANSIENT FIELD PROBLEMS

by L. E. Goodrich

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SOMMAIRE

On propose une généralisation de la méthode à intervalles de temps discrets et à moindres carrés de Zienkiewicz et de Lewis. La méthode est appliquée à un problème simple à valeurs initiales pour toute une gamme de valeurs de paramètres et la performance est comparée à celle de plusieurs méthodes bien connues. On montre que l'exactitude de la solution est supérieure à celle de la méthode de Zienkiewicz et de Lewis pour des intervalles de temps intermédiaires. Pour une valeur particulière assignée au paramètre, on obtient une méthode qui n'oscille pas peu importe l'intervalle de temps choisi. Cette méthode possède néanmoins une erreur de troncation presque comparable à celle de la méthode de Crank-Nicholson et devrait être utile pour le traitement des systèmes rigides.

On élabore aussi une méthode à moindres carrés à triple intervalle de temps et on la compare à d'autres méthodes de résolution des problèmes à valeurs initiales. La méthode ne semble pas offrir d'avantages sur les méthodes à double intervalle de temps.

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EVALUATION OF LEAST SQUARES TIME STEPPING PROCEDURES FOR TRANSIENT FIELD PROBLEMS

L.E. Goodrich*

ABSTRACT

A generalization of Zienkiewicz and Lewis's least squares time stepping procedure is proposed. The method is applied to a simple initial value problem for a range of parameter values and the performance is compared with that of several well-known methods. It is shown that solution accuracy even greater than that of Zienkiewicz and Lewis's method can be obtained for intermediate step lengths. For a particular choice of parameter value a method is obtained that will not oscillate regardless of step length chosen. This method nevertheless possesses truncation error nearly comparable to that of the Crank-Nicholson scheme and should prove useful in treating stiff systems.

A three-time-level least squares scheme is also developed and compared with other methods for the initial value problem. The method does not appear to offer any advantages over two-time-level methods.

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INTRODUCTION

For the least squares time stepping procedure finite elements in time are introduced and the square of the residual of the equation is minimized with respect to the vector of unknowns at the advanced time level. Spatial discretization of the heat conduction equation yields the system of ordinary differential equations

$$C\dot{T} + KT = 0 \tag{1}$$

where C and K are the capacitance and conductance matrices, T is the vector of instantaneous nodal temperatures, and the dot signifies time differentiation.

Defining a_j to be the nodal temperature vector at local time level j, then

$$T = \sum_{j=1}^{k} a_j N_j(s) \tag{2}$$

where N_j are the shape functions and k is the advanced time level.

Assuming that the time element is divided into k - 1 intervals Δt, the dimensionless local time is

$$s = \frac{t - t_j}{(k-1)\Delta t} \tag{3}$$

With the definitions of equations (1), (2) and (3) the least squares time stepping procedure for the heat conduction equation leads to

$$\frac{\partial \Pi}{\partial a_k} = 2 \int_0^1 ds \left\{ C\dot{N}_k + KN_k \right\}^T \cdot \left\{ \sum_{j=1}^{k} (C\dot{N}_j + KN_j) \right\} = 0 \tag{4}$$

Assuming C and K constant during Δt, and taking linear shape functions

$$N_2 = s, \; N_1 = 1-s \tag{5}$$

where $s = t/\Delta t$, leads to

$$\left(\frac{-C^T C}{\Delta t^2} + \frac{C^T K - K^T C}{2} + \frac{1}{6} K^T K \right) a_1 + \left(\frac{C^T C}{\Delta t^2} + \frac{C^T K + K^T C}{2} + \frac{1}{3} K^T K \right) a_2 = 0 \tag{6}$$

which is the equation described by Zienkiewicz and Lewis [1].

As pointed out by Lewis and Bruch [2], equation (6) has truncation error almost $O(\Delta t^3)$, which is nearly one order better than that of the Crank-Nicholson central difference scheme. Since somewhat more computation per time step is required for the least squares scheme than for the Crank-Nicholson scheme, the method is only practical if it is possible to use a larger step length. For both methods an upper limit is imposed by the existence of a critical step length beyond which the solution will oscillate, resulting in degradation of accuracy. This limit is only slightly greater for equation (6) than for the Crank-Nicholson method. The purpose of this paper is to show that a simple generalization of Zienkiewicz and Lewis's formula can be devised that gives complete control over the oscillation limit. As with the well-known "θ-method" it results in improved accuracy for intermediate step lengths and in the limit makes it possible to eliminate the oscillation altogether.

MODIFIED LEAST SQUARES IN TIME

A possible way to generalize equation (6) is to leave the shape function unspecified except for the usual normalization requirements, which imply, for two-time-levels

$$N_1 + N_2 = 1$$

and

$$N_1(0) = N_2(1) = 1$$

$$N_1(1) = N_2(0) = 0$$

Defining

$$\alpha = \Delta t^2 \int_0^1 \dot{N}_2^2 \, ds$$

$$\beta = \int_0^1 N_2 \, ds$$

$$\gamma = \int_0^1 N_2^2 \, ds$$

then equation (4) gives

$$\left[-\alpha\frac{C^TC}{\Delta t^2} + \frac{C^TK-K^TC}{2\Delta t} + (\beta-\gamma)K^TK\right]a_1 + \left[\alpha\frac{C^TC}{\Delta t^2} + \frac{C^TK+K^TC}{2\Delta t} + \gamma\, K^TK\right]a_2 = 0 \quad (7)$$

Plausible shape functions include delta functions as well as

the usual linear function, and in all such cases α must equal 1. As well, β may be set to $\frac{1}{2}$. Then equation (7) reduces to

$$\left[\frac{-C^TC}{\Delta t^2}+\frac{C^TK-K^TC}{2\Delta t}+(\tfrac{1}{2}-\gamma)K^TK\right]a_1+\left[\frac{C^TC}{\Delta t}+\frac{C^TK+K^TC}{2\Delta t}+\gamma\ K^TK\right]a_2=0 \qquad (8)$$

To establish the useful range of values for the parameter γ it suffices to consider the uncoupled modal equation, and it is only necessary to examine the simplest case obtained by replacing the matrices C and K by (scalor) unity.

$$(1+\Delta t+\gamma\Delta t^2)y_2+(-1+(\tfrac{1}{2}-\gamma)\Delta t^2)y_1=0 \qquad (9)$$

The corresponding differential equation reduces to the initial value problem

$$dy/dt=-y \quad \text{with} \quad y(o)=1 \qquad (10)$$

Stability of equation (9) is ensured for all Δt provided $|\lambda|<1$ where $\lambda=y_2/y_1$ is the characteristic equation.

For equation (9)

$$\lambda=\frac{1-(\frac{1}{2}-\gamma)\Delta t^2}{1+\Delta t+\gamma\Delta t^2} \qquad (11)$$

Imposing $\lambda>-1$ implies

$$(2\gamma-\tfrac{1}{2})\Delta t^2+\Delta t+2>0 \qquad (12)$$

which is satisfied for all Δt provided that

$$\gamma\geq\tfrac{1}{4}\,. \qquad (13)$$

For $\lambda<0$, oscillation will occur and from equation (11) the critical step length beyond which oscillation sets in is

$$\Delta t_{crit}\geq\sqrt{\frac{1}{\frac{1}{2}-\gamma}}\,. \qquad (14)$$

From equation (14), oscillation will be eliminated for all Δt if

$$\gamma=\tfrac{1}{2} \qquad (15)$$

Since the choice $\gamma=1/3$ is already optimal as regards truncation error, lesser values of γ offer no advantage at all (for $\gamma=\frac{1}{4}$, equation (9) reduces exactly to the central difference formula). It is suggested, therefore, that the best choice of γ lies in the range

$$1/3\leq\gamma\leq1/2 \qquad (16)$$

the higher values being used to avoid oscillation and thus maintain accuracy in cases of large step length.

In Figure 1 the characteristic coefficient λ is shown as a function of step length for the generalized least squares scheme of equation (11). For comparison, the characteristic coefficient

$$\lambda' = \frac{1 - (1-\theta)\Delta t}{1 + \theta\Delta t} \tag{17}$$

for the θ-method is given in Figure 2. The true solution $e^{-\Delta t}$ is represented by the solid curve in both figures.

As expected, the least squares schemes provide a much better representation of λ than do the corresponding schemes of the θ-method. Furthermore, for intermediate step lengths (say, $1 < \Delta t < 5$) the least squares method gives more accurate results if $\gamma = 4/10$ than if $\gamma = 1/3$, even though the latter value corresponds to the best truncation error. This behaviour is similar to that of the θ-method, where the Crank-Nicholson scheme can be inferior to the linear Galerkin scheme ($\theta = 2/3$) in spite of its lower truncation error. For very large step lengths the least squares scheme with $\gamma = \frac{1}{2}$ is the only one that avoids oscillation. It is clearly a considerable improvement over the backward difference scheme ($\theta = 1$) and, in fact, represents λ with an accuracy superior to that of the central difference scheme ($\theta = \frac{1}{2}$) for $\Delta t > \sim 0.9$.

In Figure 3 the truncation error for the least squares and central difference schemes is shown for the initial value problem, equation (10) for a step length $\Delta t = 1$, and with the solution started from the true value at the first step. As expected from the preceding examination of the characteristic equation, the best results are obtained for $\gamma = 4/10$, and for $\gamma = \frac{1}{2}$ the truncation error is no worse than that of the central difference scheme.

THREE-TIME-LEVEL LEAST SQUARES IN TIME

Setting $k = 3$ and taking the shape functions to be the Lagrange polynomials

$$\begin{aligned} N_1 &= 1 - 3s + 2s^2 \\ N_2 &= 4s - 4s^2 \\ N_3 &= -s + 2s^2 \end{aligned} \tag{18}$$

where $s = t/2\Delta t$,
equation (4) gives

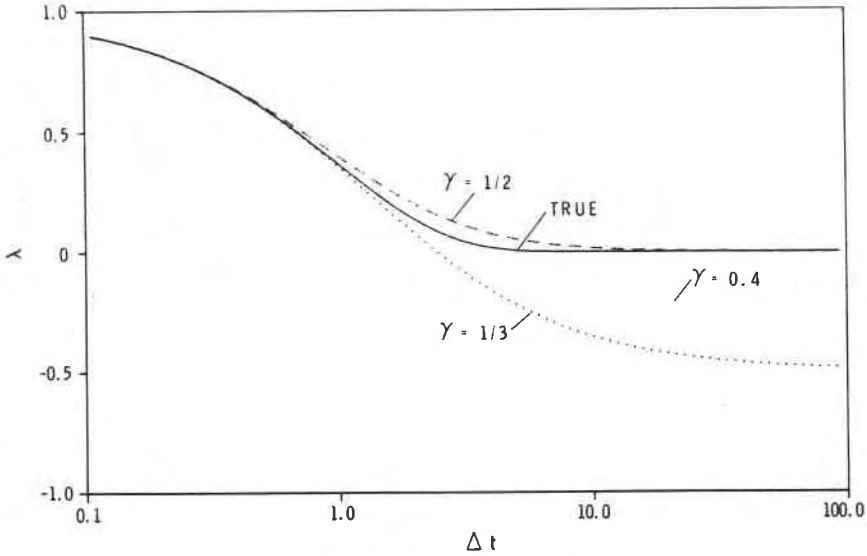

FIGURE 1
TWO-TIME-LEVEL LEAST SQUARES

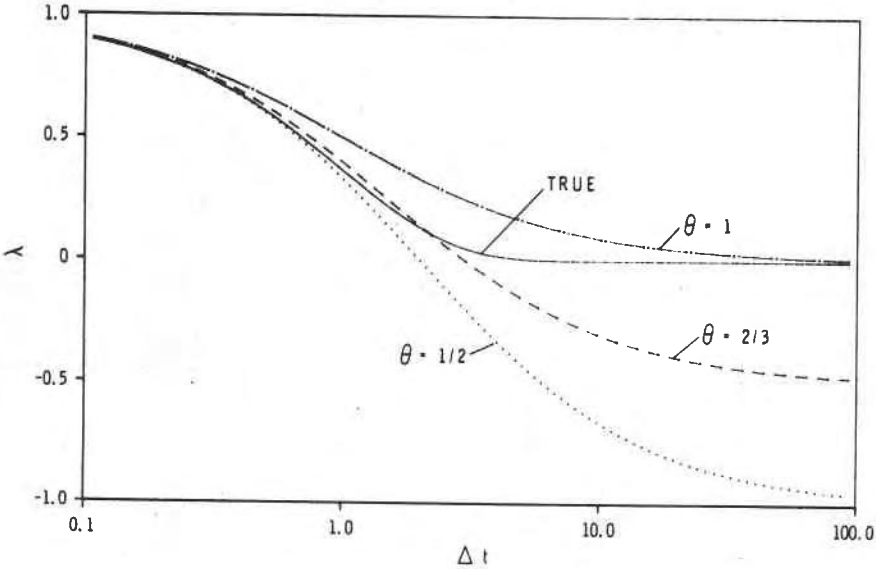

FIGURE 2
THETA METHOD

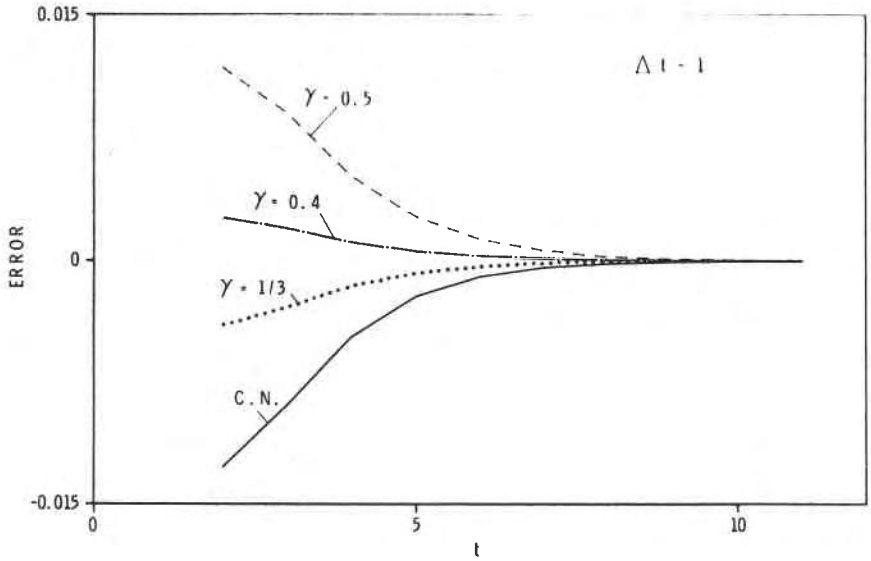

FIGURE 3
COMPARISON OF TRUNCATION ERROR

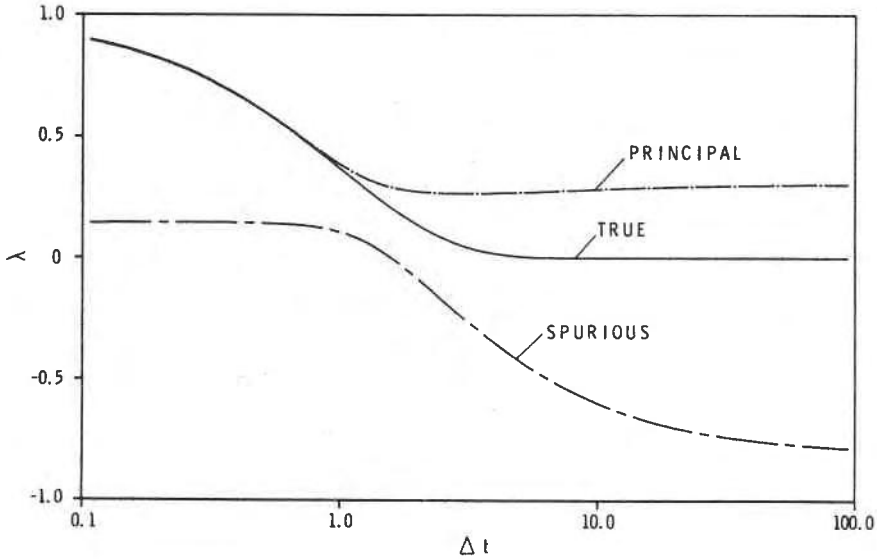

FIGURE 4
THREE-TIME-LEVEL LEAST SQUARES

$$\left(\frac{7}{2}\frac{C^TC}{\Delta t^2} + \frac{3}{2\Delta t}(C^TK + K^TC) + \frac{12}{15}K^TK\right) a_3$$

$$+ \left(\frac{-4}{\Delta t^2}C^TC + \frac{2}{\Delta t}(C^TK - K^TC) + \frac{6}{15}K^TK\right) a_2$$

$$+ \left(\frac{1}{2\Delta t^2}C^TC - \frac{1}{2\Delta t}(C^TK - K^TC) - \frac{3}{15}K^TK\right) a_1 = 0 \qquad (19)$$

The characteristic polynomial for the associated initial value problem is

$$\left(\frac{7}{2} + 3\Delta t + \frac{4}{5}\Delta t^2\right)\lambda^2 + \left(-4 + \frac{2}{5}\Delta t^2\right)\lambda + \left(\frac{1}{2} - \frac{1}{5}\Delta t^2\right) = 0 \qquad (20)$$

The two roots of equation (20)

$$\lambda = \frac{4 - \frac{2}{5}\Delta t^2 \pm \sqrt{9 - 6\Delta t - 2\Delta t^2 + \frac{12}{5}\Delta t^3 + \frac{4}{5}\Delta t^4}}{7 + 6\Delta t + \frac{8}{5}\Delta t^2} \qquad (21)$$

are both real and positive for all $\Delta t > 0$. The principal root, corresponding to the positive sign, is the approximation for the analytic value $e^{-\Delta t}$. For the method to be relatively stable the spurious root must be smaller in magnitude than the principal root. Both roots are shown in Figure 4. From the nature of their behaviour it can be inferred that the three-level-method will be unsatisfactory unless the step length is suitably small. Although not visible in the figure, the numerical results indicated that the three-level-method is superior to Zienkiewicz and Lewis's [1] two-level-method only if $\Delta t < 0.6$. Figure 5 repeats the calculation for the problem of Figure 3 and confirms the relatively unsatisfactory performance of the three-level least squares procedure.

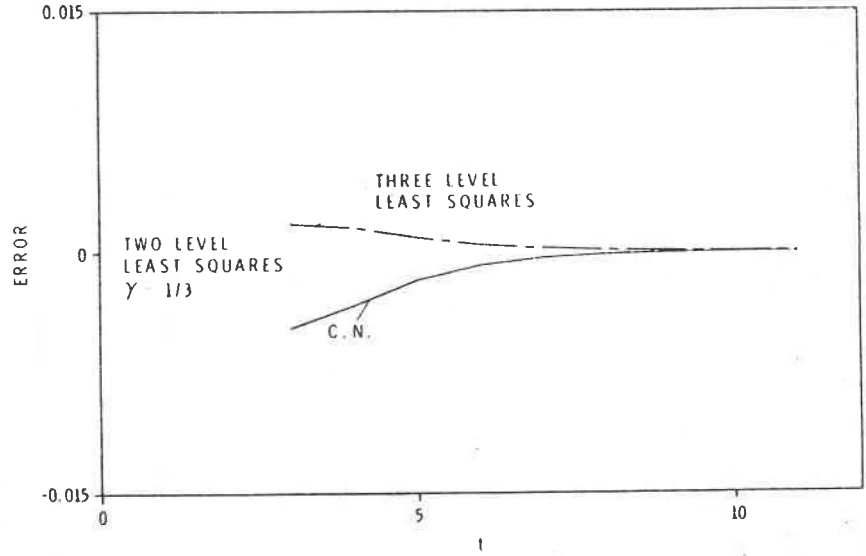

Figure 5

Comparison of truncation error for three-time-level method

CONCLUSION

A simple generalization is given for the Zienkiewicz and Lewis two-level least squares time stepping scheme for the heat conduction equation. The modified scheme has improved oscillation characteristics. This leads, in turn, to improved solution accuracy for intermediate to large step lengths.

A three-level least squares time stepping procedure is also considered. The method is more accurate than the two-level scheme only for relatively short step lengths.

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