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Goodrich, L. E.

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by L.E. Goodrich

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SOMMAIRE

Les méthodes par élément fini et par différence finie utilisées pour résoudre les problèmes de transfert de chaleur et de masse traitent habituellement la dérivée par rapport au temps en se basant sur des calculs en deux points du temps. Dans les problèmes de gel et de dégel, les équations sont non linéaires. L'absence de linéarité est due à la dépendance des propriétés du matériau sur la température et l'humidité. Avec la méthode des calculs en deux points du temps, il faut habituellement procéder par itération, afin d'obtenir des résultats précis.

Pour les situations non linéaires de ce type, on peut s'exempter du processus d'itération en utilisant un calcul en trois points du temps, dans lequel on évalue les propriétés du matériau au point intermédiaire. Le calcul le plus connu de ce type est cependant sujet à oscillation, ce qui restreint grandement son utilité.

Le présent document traite d'une nouvelle méthode de calcul en trois points du temps et la compare, en ce qui a trait à la précision et à la susceptibilité à l'oscillation, avec plusieurs autres méthodes de calculs basées sur la variation regulière par rapport au temps.

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THREE-TIME-LEVEL METHODS FOR THE NUMERICAL SOLUTION OF SOIL FREEZING PROBLEMS

L.E. Goodrich
Geotechnical Section, Division of Building Research, National Research Council of Canada (Ottawa)

ABSTRACT

Finite element and finite difference methods for heat and mass transfer problems are usually based on two-time-level schemes for treating the time derivative. In freezing and thawing problems the equations are non-linear. The non-linearity arises because of the dependence of the material properties on both temperature and moisture fields. With two-time-level schemes it is usually necessary to iterate the solution in order to obtain accurate results.

For non-linear problems of this type iteration can be avoided by using a three-time-level scheme with material properties evaluated at the intermediate time level. The most well known three-time-level scheme is, however, subject to oscillation which seriously limits its usefulness.

This paper discusses a new three-time-level scheme and compares it with several other time marching schemes from the standpoint of accuracy and susceptibility to oscillation.

For non-linear heat flow problems such as occur in freezing and thawing soils, spatial discretization using either finite elements or finite differences leads to the system of equations

$$[C]\{\dot{\theta}\} + [K]\{\theta\} = 0 \qquad (1)$$

where $\{\theta\}$ is the vector of nodal temperatures, $\{\dot{\theta}\}$ represents time derivatives and the thermal capacitance, and conductance matrices $[C]$ and $[K]$ are temperature dependent. The most widely used time-stepping procedure is the Crank-Nicholson central time difference scheme:

$$[C]\{\theta\}^{m+1} - [C]\{\theta\}^{m} + [K]\frac{\Delta t}{2}\{\theta\}^{m+1} + [K]\frac{\Delta t}{2}\{\theta\}^{m} = 0 \qquad (2)$$

While the simplest procedure to accommodate temperature-dependent thermal properties is to update the coefficient matrices at the beginning of each time step using the known thermal properties from the old time level, to ensure accuracy and convergence it is preferable to use values $[C]^{m+1/2}$ and $[K]^{m+1/2}$, determined at an intermediate time level. Because the thermal properties are functions of the unknown temperatures, $\{\theta\}^{m+1}$, iteration is required for solution. It is generally conceded that, for one- and two-dimensional linear heat flow problems, direct solution techniques are more efficient.

Direct solution methods can be retained for non-linear problems by using a three-time-level formulation in which the thermal properties are evaluated at the intermediate time level. A well known three-time-level scheme (Douglas 1961) consists in replacing the time derivative in eqn. (1) by a difference over two-time steps, while the

temperature vector is replaced by a simple average of values at three-time levels, viz.,

$$[C]\{\theta\}^{m+1} - [C]\{\theta\}^{m-1} + \frac{2\Delta t}{3}[K]\left(\{\theta\}^{m+1} + \{\theta\}^{m} + \{\theta\}^{m-1}\right) = 0 \qquad (3)$$

This method has been used with finite difference schemes by Bonacina and Comini (1973) and Bonacina et al (1973). A finite element formulation for heat transfer with phase change is described in Comini et al (1974). Although eqn. (3) is unconditionally stable, the method is subject to serious oscillations. Comini and Lewis (1976) describe an averaging procedure that is helpful in controlling the oscillation but that does not eliminate it.

A general method of formulating multi-time level marching methods using finite elements in time is outlined in Zienkiewicz (1971). Assuming an interpolated form for the time-dependent temperature vector

$$\{\theta\} = \sum_{j=m-n}^{m+1} N^{j}(t)\{\theta\}^{j} \qquad (4)$$

where $\{\theta\}^{j}$ is the nodal temperature vector at time level j, and $N^{j}(t)$ are shape functions in time, then applying the Galerkin weighted residual procedure to eqn. (1) gives

$$\int_{t^{m-n}}^{t^{m+1}} N^{m+1}(t)\left[[C]\{\dot{\theta}\} + [K]\{\theta\}\right]dt = 0 \qquad (5)$$

Only one weighted residual equation is required because the temperatures are known at time levels $j \leq m$.

Using quadratic Lagrange polynomials as shape functions leads to a three-time-level formulation. In terms of the local time $\tau = t - t^{m-1}$, the element shape functions are

$$N^{m-1} = \frac{(\Delta_1-\tau)(\Delta_1+\Delta_2-\tau)}{\Delta_1 \cdot (\Delta_1+\Delta_2)} \qquad (6a)$$

$$N^{m} = \frac{\tau \cdot (\Delta_1+\Delta_2-\tau)}{\Delta_1 \cdot \Delta_2} \qquad (6b)$$

$$N^{m+1} = \frac{\tau(\tau-\Delta_1)}{\Delta_2 \cdot (\Delta_1+\Delta_2)} \qquad (6c)$$

where $\Delta_1 = t^{m} - t^{m-1}$, and $\Delta_2 = t^{m+1} - t^{m}$.

Combining eqns. (4), (5) and (6) and assuming that [C] and [K] are independent of time in the interval $t^{m-1} \leq t \leq t^{m+1}$, yields

$$[C]\left[(\alpha-3)\{\theta\}^{m-1} - \alpha\{\theta\}^{m} + 3\{\theta\}^{m+1}\right] + \frac{\Delta_1+\Delta_2}{10} \cdot [K]\left[(10-3\alpha)\{\theta\}^{m-1} + (3-2\delta)\alpha \cdot \{\theta\}^{m} + 2(\delta\alpha-5(\delta-1))\{\theta\}^{m+1}\right] = 0 \qquad (7)$$

where $\delta = \Delta_1/\Delta_2$, and $\alpha = (1+\delta) \cdot (1+1/\delta)$.

For a fixed time step $\Delta_1 = \Delta_2 = \Delta t$, eqn. (7) reduces to

$$[C]\left[\{\theta\}^{m-1} - 4\{\theta\}^{m} + 3\{\theta\}^{m+1}\right] + \frac{2\Delta t}{5} \cdot [K]\left[-\{\theta\}^{m-1} + 2\{\theta\}^{m} + 4\{\theta\}^{m+1}\right] = 0 \qquad (8)$$

Figure 1 illustrates the behaviour of the truncation error of the quadratic Galerkin three-time-level scheme, eqn. (8), compared with that for several other schemes. The problem considered is that of one-dimensional heat conduction in an homogeneous semi-infinite medium initially isothermal at zero temperature and whose surface is suddenly brought to temperature -1. The grid spacing, time step and thermal diffusivity values assumed are indicated on the figure and correspond to $\alpha\Delta t/\Delta x^2 = 2.58$. In all cases the numerical solution was started at time level $3\Delta t$ using the analytical solution to generate temperature values at time levels Δt, $2\Delta t$. The figure shows the over-all error for the first interior node point.

As seen in Fig. 1(a), the method of eqn. (3) results in very large oscillations. Although stable, oscillation of this magnitude could lead to serious errors in problems with time dependent boundary conditions or with temperature dependent

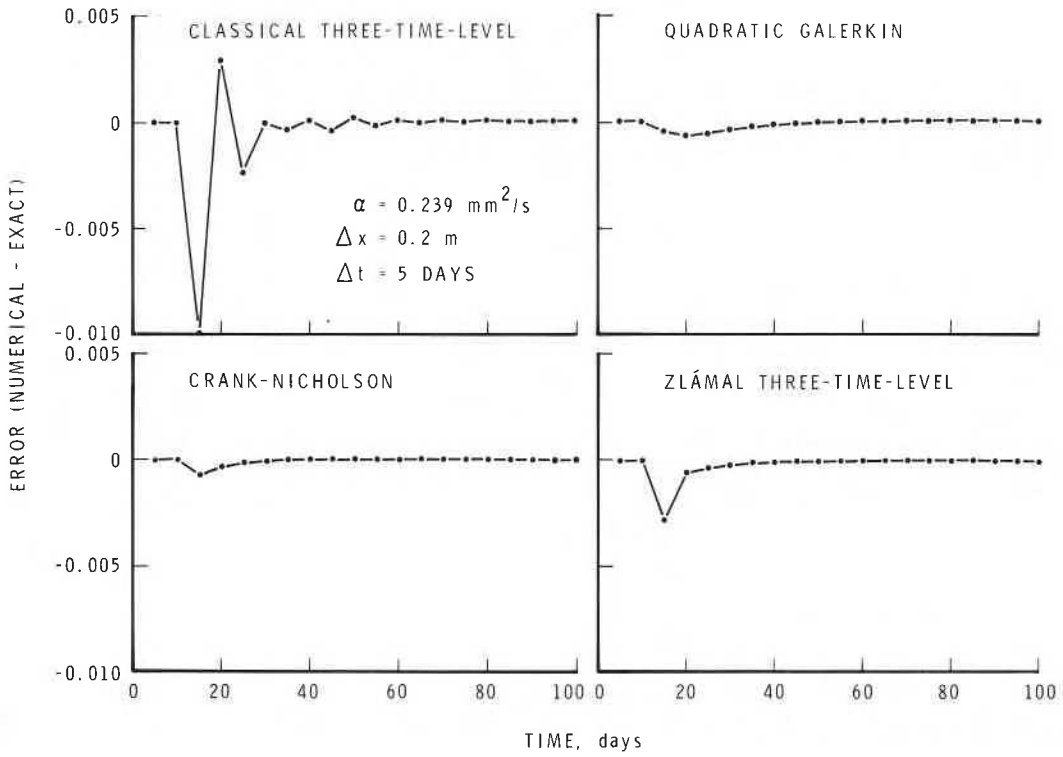

Fig. 1. Truncation error for a simple heat flow problem.

thermal properties. The quadratic Galerkin scheme, eqn. (8), gives results shown in Fig. 1(b) similar to those of the Crank-Nicholson scheme, Fig. 1(c). The quadratic Galerkin method does, however, exhibit slightly greater errors than those of eqn. (2) during the first few time steps. Results for a three-time-level scheme proposed by Zlámal (1975) are shown in Fig. 1(d). Although the error of Zlámal's scheme is slightly superior to that of the quadratic Galerkin scheme for intermediate times, relatively larger errors occur at early times with Zlámal's method. Both Zlámal's scheme and the quadratic Galerkin scheme are distinctly superior to the three-time-level scheme of eqn. (3). Because the quadratic Galerkin scheme produces a more smoothly varying truncation error, it may give more accurate over-all results than Zlámal's scheme when applied to practical problems with temperature dependent thermal properties.

In order to verify the performance of the quadratic Galerkin scheme with variable time steps, eqn. (7) was applied to the sample problem of Fig. 1, using a ratio of successive time steps $\Delta t^{m+1}/\Delta t^{m} = 1.1$. This corresponded to an increase in the parameter $\alpha\Delta t/\Delta x^2$ from 2.58 to 21.0 after 24 time steps. The results, shown in Fig. 2, indicate that the quadratic Galerkin variable time step scheme is satisfactory. The truncation error is, however, somewhat larger than that of the Crank-Nicholson scheme.

Zlámal's scheme is obtained from the general two-step method

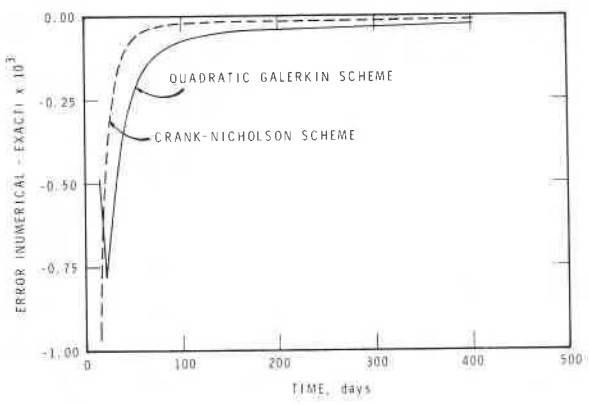

Fig. 2. Truncation error with increasing time step.

$$[C] \sum_{j=-1}^{+1} \alpha_j \{\theta\}^{m+j} + [K]\,\Delta t \sum_{j=-1}^{+1} \beta_j \{\theta\}^{m+j} = 0 \qquad (9)$$

with coefficients α_j, β_j chosen so as to minimize the maximum modulus of the roots of the characteristic equation. In this way the stability of the scheme for large time steps should be improved.

In terms of the Zienkiewicz two-parameter three-time-level scheme described in Wood (1978)

$$[C]\left\{\alpha\{\theta\}^{m+1} + (1-2\alpha)\{\theta\}^{m} + (\alpha-1)\{\theta\}^{m-1}\right\}$$

$$+ [K]\,\Delta t \left\{\beta\{\theta\}^{m+1} + \tfrac{1}{2}(1 + 2\alpha - 4\beta)\{\theta\}^{m}\right.$$

$$\left. + \tfrac{1}{2}(1 - 2\alpha + 2\beta)\{\theta\}^{m-1}\right\} = 0 \qquad (10)$$

Zlámal's scheme corresponds to

$$\alpha = \tfrac{1}{2} + \sigma$$
$$\beta = \tfrac{1}{4}(1 + \sigma)^2 \qquad (11)$$
$$0 < \sigma \leq 1$$

which, with $\sigma = 1/3$ as recommended by Zlámal, gives,

$$\alpha = 5/6$$
$$\beta = 4/9 \qquad (12)$$

By inspection, eqn. (8) also corresponds to eqn. (10) but with

$$\alpha = 3/2$$
$$\beta = 4/5 \qquad (13)$$

In the notation of Wood (1978), eqn. (10) is A_o stable if $\alpha \geq \tfrac{1}{2}$ and $\beta > \alpha/2$. The method is second order with error coefficient

$$C = -1(1/12 + \beta - \alpha/2) \qquad (14)$$

Thus the quadratic Galerkin scheme, eqn. (8), is A_o stable but the error coefficient is

$$C = -(1/12 + 1/20)$$

while for Zlámal's scheme, with $\sigma = 1/3$,

$$C = -(1/12 + 1/36)$$

Woods (1978) compared the behaviour of several multi-level schemes for the pure initial value problem

$$\frac{dy}{dt} = -y\,; \quad y(o) = 1 \qquad (15)$$

and concluded that Zlámal's scheme was subject to unacceptable oscillation at large values of step length. Wood's numerical experiments were repeated and the results are summarized in Table 1. Table 1(a) for step length $\Delta t = 0.5$ shows Zlámal's scheme to be inferior to the quadratic Galerkin scheme for the first three steps. The superior truncation error of Zlámal's scheme does, however, show up at subsequent steps. Table 1(b) shows the results when the step length is increased to $\Delta t = 5.0$. In this case the quadratic Galerkin scheme produces results with a distinctly smaller oscillation than that of Zlámal's scheme. As a result, the over-all error is also considerably better for the quadratic Galerkin scheme.

Table 1 also contains results calculated using the "classical" three-time-level method (eqn. (3)) with smoothing as recommended by Comini and Lewis (1976). Although smoothing is helpful for $\Delta t = 0.5$, for $\Delta t = 5.0$ the truncation error and oscillation are nearly as bad with as without smoothing. In all

TABLE 1(a)

Comparison of errors for various one- and two-step methods $\Delta t = 0.5$

t	Exact $y=e^{-t}$	Error (Numerical - Exact) for 1-step methods		
		Backward Difference	Crank-Nicholson	Linear Galerkin
1.0	3.679E-01	3.647E-02	-3.961E-03	1.120E-02
1.5	2.231E-01	4.644E-02	-4.779E-03	1.380E-02
2.0	1.353E-01	4.438E-02	-4.325E-03	1.274E-02
2.5	8.208E-02	3.772E-02	-3.479E-03	1.046E-02
3.0	4.979E-02	3.009E-02	-2.623E-03	8.056E-03
3.5	3.020E-02	2.305E-02	-1.899E-03	5.955E-03
4.0	1.832E-02	1.718E-02	-1.337E-03	4.279E-03
4.5	1.111E-02	1.256E-02	-9.216E-04	3.013E-03
5.0	6.738E-03	9.039E-03	-6.255E-04	2.088E-03

t	Exact $y=e^{-t}$	Error (Numerical - Exact) for 2-step methods			
		Classical	Comini and Lewis	Zlámal	Quadratic Galerkin
1.0	3.679E-01	-1.951E-02	-1.951E-02	-7.235E-03	-3.799E-03
1.5	2.231E-01	-6.957E-03	1.559E-02	-7.435E-03	-5.901E-03
2.0	1.353E-01	-1.519E-02	1.144E-02	-6.553E-03	-6.188E-03
2.5	8.208E-02	-4.033E-03	1.429E-02	-5.156E-03	-5.468E-03
3.0	4.979E-02	-9.230E-03	1.100E-02	-3.840E-03	-4.391E-03
3.5	3.020E-02	-1.311E-03	9.093E-03	-2.754E-03	-3.321E-03
4.0	1.832E-02	-5.259E-03	6.704E-03	-1.924E-03	-2.410E-03
4.5	1.111E-02	7.002E-05	4.968E-03	-1.318E-03	-1.699E-03
5.0	6.738E-03	-3.004E-03	3.536E-03	-8.901E-04	-1.172E-03

TABLE 1(b)

Comparison of errors for various one- and two-step methods $\Delta t = 5.0$

t	Exact $y=e^{-t}$	Error (Numerical - Exact) for 1-step methods		
		Backward Difference	Crank-Nicholson	Linear Galerkin
10.0	4.540E-05	1.078E-03	-2.933E-03	-1.082E-03
15.0	3.059E-07	1.869E-04	1.237E-03	1.592E-04
20.0	2.061E-09	3.119E-05	-5.304E-04	-2.454E-05
25.0	1.389E-11	5.199E-06	2.273E-04	3.775E-06
30.0	9.358E-14	8.665E-07	-9.742E-05	-5.807E-07
35.0	6.305E-16	1.444E-07	4.175E-05	8.934E-08
40.0	4.248E-18	2.407E-08	-1.789E-05	-1.374E-08
45.0	2.863E-20	4.012E-09	7.669E-06	2.115E-09
50.0	1.929E-22	6.686E-10	-3.287E-06	-3.253E-10

t	Exact $y=e^{-t}$	Error (Numerical - Exact) for 2-step methods			
		Classical	Comini and Lewis	Zlámal	Quadratic Galerkin
10.0	4.540E-05	-5.437E-01	-5.437E-01	-1.307E-01	9.086E-02
15.0	3.059E-07	4.146E-01	3.351E-01	6.568E-02	6.122E-04
20.0	2.061E-09	-2.616E-02	-2.480E-01	-1.680E-02	8.264E-03
25.0	1.389E-11	-2.031E-01	1.784E-01	1.948E-04	5.569E-05
30.0	9.358E-14	1.703E-01	1.289E-01	2.039E-03	7.513E-04
35.0	6.305E-16	-2.165E-02	9.302E-02	-1.063E-03	5.062E-06
40.0	4.248E-18	-7.505E-02	-6.716E-02	2.816E-04	6.830E-05
45.0	2.863E-20	6.939E-02	4.848E-02	-8.076E-06	4.602E-07
50.0	1.929E-22	-1.297E-02	-3.500E-02	-3.173E-05	6.209E-06

cases the method remains distinctly inferior to both Zlámal's and the quadratic Galerkin scheme.

CONCLUSION

The quadratic Galerkin three-time-level scheme presented here is distinctly superior to the usual three-time-level scheme as regards to both oscillation and truncation error. Although the truncation error is slightly greater than that for a similar method proposed by Zlámal, the quadratic Galerkin method remains usable over a larger range of step lengths and, for this reason, should be more attractive for practical applications.

REFERENCES

Bonacina, C. and Comini, G. (1973), On the solution of the nonlinear heat conduction equations by numerical methods, Int. J. Heat Mass Transfer, 16: 581-589.

Bonacina, C., Comini, G., Fasano, A. and Primicerio, M. (1973), Numerical solution of phase-change problems, Int. J. Heat Mass Transfer, 16: 1825-1832.

Comini, G., Del Guidice, S., Lewis, R.W., and Zienkiewicz, O.C. (1974), Finite element solution of non-linear heat conduction problems with special reference to phase change, Int. J. Num. Meth. Eng., 8: 613-624.

Comini, G. and Lewis, R.W. (1976), A numerical solution of two-dimensional problems involving heat and mass transfer, Int. J. Heat Mass Transfer, 19: 1387-1392.

Douglas J. (1961), A survey of numerical methods for parabolic differential equations in Advances in Computers, Academic Press, New York, Vol. 2, pp. 1-54.

Wood, W.L. (1978), On the Zienkiewicz three- and four-time-level schemes applied to the numerical integration of parabolic equations, Int. J. Num. Meth. Eng., 12: 1717-1726.

Zienkiewicz, O.C. (1971), The finite element in engineering science, McGraw-Hill, London, 521 p.

Zlámal, M. (1975), Finite element methods in heat conduction problems, Proc. Conf. Finite Element Methods, Brunel University, pp. 85-104.