An Appraisal of Computational Techniques for Transient Heat Conduction Equation

T. Kant

Civil Engineering Department, Indian Institute of Technology (IIT), Bombay-400 076, India

SUMMARY

A semi-discretization procedure in which the 'space' dimension is discretized by the finite element method is emphasized for transient problems. This standard methodology transforms the space-time partial differential equation (PDE) system into a set of ordinary differential equations (ODE) in time. Existing methods for transient heat conduction calculations are then reviewed. Existence of two general classes of time integration schemes- implicit and explicit is noted. Numerical stability characteristics of these two methods are elucidated. Implicit methods are noted to be numerically stable, permitting large time steps, but the cost per step is high. On the otherhand, explicit schemes are noted to be inexpensive per step, but small step size is required. Low computational cost of the explicit schemes make it very attractive for nonlinear problems. However, numerical stability considerations requiring use of very small time steps come in the way of its general adoption. Effectiveness of the fourth-order Runge-Kutta-Gill explicit integrator is then numerically evaluated. Finally we discuss some very recent works on development of computational algorithms which not only achieve unconditional stability, high accuracy and convergence but involve computations on matrix equations of elements only. This development is considered to be very significant in the light of our experience gained for simple heat conduction calculations. We conclude that such algorithms have the potential for further developments leading to development of economical methods for general transient analysis of complex physical systems.

*The author wishes to express his gratitude to Professor O.C. Zienkiewicz who introduced him to this fascinating area of research and especially the FEE scheme.

1. INTRODUCTION

We consider here the time-dependent general quasi-harmonic equation,

$$c\frac{\partial\phi}{\partial t} = \frac{\partial}{\partial x}(k_x\frac{\partial\phi}{\partial x}) + \frac{\partial}{\partial y}(k_y\frac{\partial\phi}{\partial y}) + \frac{\partial}{\partial z}(k_z\frac{\partial\phi}{\partial z}) + Q \qquad \ldots (1)$$

which is to be solved for the field variable $\phi(\underset{\sim}{x},t)$ in a solution domain Ω bounded by surface Γ, with the boundary conditions (t>0),

$$\phi(\underset{\sim}{x},\ t) = \bar{\phi} \text{ on} \qquad \text{and} \quad -(k\nabla\phi)^T\hat{n} = \bar{q} \text{ on } \Gamma_2 \qquad \ldots (2)$$

such that the union of Γ_1 and Γ_2 forms the complete boundary Γ. Because the problem is time-dependent, and (1) has a first derivative in time, an initial condition on ϕ in the form of,

$$\phi\ (\underset{\sim}{x},\ 0) = \phi_o \text{ in } \Omega \qquad \ldots (3)$$

is required to complete the problem definition.

If a semi-discretization procedure is adopted and the space $\underset{\sim}{x}$ is discretized by the finite element method in the usual manner with the assumption of the trial function of the type,

$$\phi \simeq \Sigma\ N_i(x)a_i(t) \qquad \ldots (4)$$

we transform (1) into a system of ordinary differential equations in time of the form,

$$\underline{C}\ \dot{\underset{\sim}{a}} + \underline{K}\ \underset{\sim}{a} + \underset{\sim}{f} = 0 \qquad \ldots (5)$$

in which

$$K_{ij} = \sum_e \int_{\Omega_e}(k_x\frac{\partial N_i}{\partial x}\frac{\partial N_j}{\partial x} + k_y\frac{\partial N_i}{\partial y}\frac{\partial N_j}{\partial y} + k_z\frac{\partial N_i}{\partial z}\frac{\partial N_j}{\partial z})d\Omega \qquad \ldots(6a)$$

$$C_{ij} = \sum_e \int_{\Omega_e} N_i\ c\ N_j\ d\Omega \qquad \ldots(6b)$$

and $$f_i = -\sum_e \int_{\Omega_e} QN_i d\Omega + \int_{\Gamma_2}\bar{q}\ N_i d\Gamma \qquad \ldots(6c)$$

For heat conduction problems $\underline{C}$ is the capacitance matrix, $\underline{K}$ is the conductivity matrix, $\underset{\sim}{f} = \underset{\sim}{f}(t)$ is the heat supply vector and $\underset{\sim}{a}$ is the nodal temperature vector. A superposed dot represents temporal (time, t) differentiation.

Provided that the boundary conditions (2) are implicit in the discrete equation (5), the initial value problem (IVP) for (5) consists in evaluating $\underset{\sim}{a} = \underset{\sim}{a}(t)$ which satisfies (5) and the initial condition

$$\underset{\sim}{a}(0) = \underset{\sim}{a}^o \qquad \ldots (7)$$

corresponding to (3). The vector $\underset{\sim}{a}^o$ here is a given vector of initial nodal parameters.

Further we can also write (5) in the general implict form

$$\underline{F}'(\underset{\sim}{a},\ t,\ \dot{\underset{\sim}{a}}) = 0 \qquad \ldots (8)$$

or in the standard explicit format

$$\dot{\underset{\sim}{a}} = \underset{\sim}{F}\ (\underset{\sim}{a},\ t) \qquad \ldots (9)$$

with

$$\underset{\sim}{F}(\underset{\sim}{a},\ t) = -\ \underset{\sim}{C}^{-1}(\underset{\sim}{K}\ \underset{\sim}{a} + \underset{\sim}{f}) \qquad \ldots (10)$$

2. AN OVERVIEW OF EXISTING METHODS

Time integration of the discrete equation (5) is carried out either by PDE or ODE integrators. Methods in either of these are classified as one-step or multistep, explicit or implicit. In the former approach time derivative is directly replaced by finite difference quotient. Such schemes are popular in the finite element literature and for a description of these, the reader should consult a standard text [1]. Alternatively, these schemes are also derived by applying Galerkin finite elements in time to discrete equation (5), we obtain recurrence relation of the type

$$(\underset{\sim}{C} + \underset{\sim}{K}\ \Delta t\ \Theta)\underset{\sim}{a}^{n+1} = (\underset{\sim}{C} - \underset{\sim}{K}\ \Delta t\ \overline{1 - \Theta})\underset{\sim}{a}^{n} - \Delta t\ \overline{\underset{\sim}{f}} \qquad \ldots (11)$$

when a linear interpolation of $\underset{\sim}{a}$ in the time interval $\Delta t = t_{n+1} - t_n$ is assumed. The term $\overline{\underset{\sim}{f}}$ represents here the weighted force term. It is noted that Euler's forward difference, Crank-Nicholson's mid-difference and the backward difference schemes are nothing but special cases of (11) for which Θ equals 0, 1/2 and 1 respectively. Further, a scheme with Galerkin type weighting for which $\Theta = 2/3$ is also obtained. For a critical review and derivation of these and other multistep schemes, one should refer Zienkiewicz [1].

The latter class of schemes belonging to ODE integrators make use of the forms (8) or (9). An extensive literature of well-understood, highly accurate and stable (?) schemes exists [2-8]. Space limitation does not permit discussion of these schemes here. We shall make use of one such scheme for our numerical experimentation - the one-step explicit fourth-order Runge-Kutta-Gill method.

We have attempted a brief overview of the various available schemes. Basically the schemes fall under two categories : implicit and explicit. Implicit schemes tend to be stable, permitting large time steps, but the cost per step is high due to system equation solving. On the other hand, explicit schemes tend to be inexpensive per step, but stability considerations require that small steps be employed. Recent efforts have been towards 'marriage' of these two approaches in one scheme. Trujillo [9] has proposed an explicit algorithm corresponding to the basic recurrence relation (11). In this $\underline{C}$ is diagonalized and $\underline{K}$ is split into some kind of lower and upper triangular forms. A step size fifteen times greater than that allowed by the conventional explicit method is claimed. Hughes, et al. [10] have recently proposed an element-by-element implicit algorithm for the discrete equation (5) with lumped $\underline{C}$. With an approximation for $\underline{K}$ as $\underset{e}{\pi}\ \underline{K}_e$ in (11), the computations proceed on an element-by-element basis. Zienkiewicz et al. [11,12] have outlined a procedure based on systematic partitioning of the discrete

equation (5) and involving extrapolation. The scheme which could utilize any one-step θ algorithm and a suitable extrapolation procedure had the potential of achieving both unconditional stability in general and explicitness of the computation in the limit. The full potential of this idea has not yet been fully explored. The motivation for the frontal extrapolated explicit (FEE) scheme [13] which is also discussed in this paper in some detail has come from these earlier works. The scheme, based on an intuitive approach, makes use of an innovative element-based computational model. This scheme with a one-step θ algorithm, turns out to be unconditionally stable and fully explicit in the limit when space discretizations are effected with linear elements.

3. MODEL PROBLEM

In order to compare the various algorithms discussed in this paper, we have chosen a one-dimensional transient heat equation [14, 15],

$$\frac{\partial \phi}{\partial t} = \frac{\partial^2 \phi}{\partial x^2} \qquad \ldots (12)$$

with boundary conditions,

$$\phi(0,t) = 1 \text{ and } \frac{\partial \phi}{\partial x}(L,t) = 0; \text{ for } t > 0 \qquad \ldots (13)$$

and initial condition,

$$\phi(x,0) = 0 \; ; \; 0 \leqslant x \leqslant L \qquad \ldots (14)$$

We note that the whole bar whose length is L, is insulated except at x=0 and hence a steady state solution is a uniform temperature of unity. This problem has an exact solution [14].

$$\phi(x,t) = 1 - \sum_{m=1}^{\infty} \frac{4}{\pi(2m-1)} \exp\left\{ - \left[\frac{(2m-1)\pi}{8}\right]^2 t \right\} \sin\left[\frac{(2m-1)\pi x}{8}\right] \qquad \ldots (15)$$

We discretize the x-dimension here by two noded linear finite elements with element matrices as,

$$\underline{K}_e = \begin{bmatrix} 1/h_e & -1/h_e \\ -1/h_e & 1/h_e \end{bmatrix} \quad \text{and} \quad \underline{C}_e = \begin{bmatrix} h_e/3 & h_e/6 \\ h_e/6 & h_e/3 \end{bmatrix} \qquad \ldots (16)$$

in which h_e is an element's length such that $L = \sum_e h_e$. The system matrices are formed in the usual manner, i.e.,

$$\underline{C} = \sum_e C_e \quad \text{and} \quad \underline{K} = \sum_e \underline{K}_e \qquad \ldots (17)$$

An estimate of the maximum time step size (Δt_{cr}) in Euler's explicit scheme is first obtained by evaluating the largest eigenvalue (frequency) λ_{max} of the eigenvalue problem,

$$\underline{K}\, \underline{a} = \underline{C}\, \underline{a} \qquad \ldots (18)$$

by making use of the theorem provided by Irons [16]. Thus,

$$|\underline{K}_e - \lambda_e \underline{C}_e| = 0 \qquad \ldots (19)$$

provides an upper bound to the eigenvalues. This turns out to be $4/h_e^2$ and thus the critical time step Δt_{cr} for Euler's scheme, $2/\lambda_{max}$ is simply

obtained as $h_e^2/2$. All the numerical computations have been performed by discretising the total length, L = 4 units, by four equal space elements and thus setting $h_e = 1 (e = 1,2,3 \text{ and } 4)$.

4. RUNGE-KUTTA-GILL ODE INTEGRATOR

The enormity of available algorithms for ODEs makes the choice a specific formula a difficult task. We have chosen here the Gill's version of the fourth-order Runge-Kutta one-step integrator [2,5] because of its proven success [6,7]. The details of the algorithms are omitted here for limitations of the space. We assume the explicit form (9) and we do not form the global matrices explicitly. Instead, we compute the $\underset{\sim}{F}$ vector in (10) by summing the element's contribution in a systematic manner. A diagonal $\underline{C}$ matrix is obtained by lumping the off-diagonal terms by a simple row sum technique. The response obtained with this scheme is presented and compared with exact solution and that obtained with Euler's scheme in Figures 1-2 at two space points.

The application of the fixed boundary value of $\phi(0,t)=1$ needs special mention. This point has been discussed extensively for PDE integrators[15] wherein full value is never imposed in one time step as it causes 'noise'. We like to emphasize that with the fourth order RKG scheme, no such noise is observed.

5. FRONTAL EXTRAPOLATED EXPLICIT (FEE) SCHEME

With reference to the recurrende relation (11), we derive the two-step computational model,

$$\underset{\sim}{F}_e = (\underline{C}^1 + \Delta t\, \underline{K}_e \Theta)\underset{\sim}{a}_{e*}^{n+1} + (-\underline{C}^1 + \Delta t \underline{K}_e\, \overline{1-\Theta})\underset{\sim}{a}_e^n \qquad \ldots (20)$$

$$(\underline{C}^1 + \Delta t \underline{K}_e \Theta)\underset{\sim}{a}_e^{n+1} = -\underset{\sim}{F}_{e+1} - (-\underline{C}^1 + \Delta t \underline{K}_e \overline{1-\Theta})\underset{\sim}{a}_e^n \qquad \ldots (21)$$

which involves only element-size matrices and vectors. A quantity with asterisk(*) represents an extrapolated value which can be as simple as $\underset{\sim}{a}_*^{n+1} \simeq \underset{\sim}{a}^n$ and this we have used in our computations. In the above only $\underline{K}$ is split element wise and the elements of $\underline{C}^1$ are those corresponding to the lumped system matrix based on diagonalization using simple row-sum technique. The first step in this scheme consists in computing the element's force vector $\underset{\sim}{F}_e$ based on extra-polated values at time step t_{n+1}, for all the elements. The solution vector at time t_{n+1} is then obtained, element-by-element by (21). The subscript $e\pm1$ refers to the force contribution coming from the adjoining elements for the element under consideration.

We present the results at space points x=1 and 2 for various time step sizes $\Delta t \geqslant \Delta t_{cr}$ by employing a value of Θ equal to 1/2, 2/3 and 1 in figures 3-8. Throughout we have compared the results of this scheme with that of the exact solution. A perusal of these results show both unconditional stability and high accuracy of the algorithm. The scheme employing $\Theta = 1/2$ is seen to be most accurate as is usual with a one-step implicit

scheme (2nd order accuracy). However, we see that it has its associated noise effects which is common with such a scheme [15] when full value of temperature is instantaneously imposed at the end x=0 at t>0. As expected, no noise phenomenon is seen with $\theta = 1$, but the results are observed to be least accurate (although are reasonably accurate for practical problems). The oscillations are seen to be very much smoothened out in this scheme with $\theta = 2/3$, which is again an established observation.

Further, all the results have been obtained with the simplest 'one-pass forward' FEE scheme in which the nodal solution advancing scheme is derived by making use of the second equation of each element. We start with the first element whose first node (boundary node) is always held at a constant temperature $\phi = 1$, and thus solve explicitly for node-2. This process is repeated for other elements in a sequencial manner.

6. CONCLUSIONS

Existing methods falling under the two broad categories, explicit and implicit are first reviewed. The results of an experiment with the fourth-order Runge-Kutta ODE integrator are then presented. From the point of view of accuracy, the method could be recommended for obtaining general transient response. However, two disappointing features of this scheme appears to have been confirmed here. These are (i) stable step size is only 30-40% greater than that for the Euler's scheme and (ii) computational cost per step is roughly four times that of Euler's scheme. A breakthrough appears to have been made and it seems possible to have schemes possessing both the explicitness/near explicitness of the computation and the desirable unconditional stability of the implicit algorithms. Efforts of ours in such a development have been mainly based on an intuitive approach. We have described one such scheme (FEE) from a class of new such schemes. The preliminary test results are very encouraging. Considerable further work remains to be done in exploring the behaviour of this and other related schemes for a variety linear and nonlinear problems. Finally, rigorous stability and accuracy analyses of these schemes need to be pursued seriously to put matters on a sound footing.

REFERENCES

[1] Zienkiewicz, O.C., The Finite Element Method, Third Edition, McGraw-Hill London, 1977.

[2] Ralston, A. and Wilf, H.S. (Editors), Mathematical Methods for Digital Computers, Vol.1, Wiley, New York, 1960.

[3] Henrici, P., Discrete Variable Methods in Ordinary Differential Equations, Wiley, New York, 1962.

[4] Lambert, J.D., Computational Methods in Ordinary Differential Equations, Wiley, London, 1973.

[5] Gill, S., 'A process for the step-by-step integration of differential equations in an automatic digital computing machine', Proc. Camb. Phil. Soc., 47, 96-108 (1951).

[6] Kant, T. and Ramesh, C.K., 'Numerical integration of linear boundary value problems in solid mechanics by segmentation method', Int. J.Num. Method Engng., 17, 1233-1256 (1981).

[7] Kant, T., 'An experiment with Runge-Kutta-Gill algorithm in finite element computations of transient heat conduction', Res. Rep. C/R/416/82, Civil Engg. Dept., University of Wales, Swansea (U.K.), 1982.

[8] Felippa, C.A. and Park, K.C., 'Computational aspects of time integration procedures in structural dynamics, Part I : Implementation', ASME Journal of Applied Mechanics, 45, 595-602 (1978).

[9] Trujillo, D.M., 'An unconditionally stable explicit algorithm for structural dynamics', Int. J. Num. Method Engng., 11, 1579-1592 (1977).

[10] Hughes, T.J.R., Levit, I. and Winget, J., 'Unconditionally stable element-by-element implict algorithms for heat conduction analysis', Proc., U.S. Applied Mechanics Conf., Cornell University, Ithaca (U.S.A.), 1982.

[11] Zienkiewicz, O.C. and Taylor, R.L., 'Some developments of the finite element methods for fluid mechanics', Proc., Third Int. Conf. on Finite Elements in Flow Problems, Alberta (Canada), 1980.

[12] Zienkiewicz, O.C., Hinton, E., Leung, K.H. and Taylor, R.L., 'Staggered time marching schemes in dynamic soil analysis and a selective explict extrapolation algorithm', Proc., Second Int. Symp. on Innovative Numerical Analysis in Applied Engg. Sciences, Canada, 1980.

[13] Zienkiewicz, O.C. and Kant, T. 'A frontal extrapolated explicit scheme for transient field problems', Res. Rep. C/R/415/82, Civil Engg. Dept., University of Wales, Swansea (U.K.), 1982.

[14] Carslaw, H.S. and Jaegar, J.C., Conduction of Heat in Solids, Oxford University Press, Oxford, 1959.

[15] Wood, W.L. and Lewis, R.W., 'A comparison of time marching schemes for the transient heat conduction equation', Int. J. Num. Method Engng., 9, 679-689 (1975).

[16] Irons, B.M., 'Application of a theorem on eigenvalues to finite element problems', Res. Rep. C/R/132/70, Civil Engg. Dept., University of Wales, Swansea (U.K.), 1970.

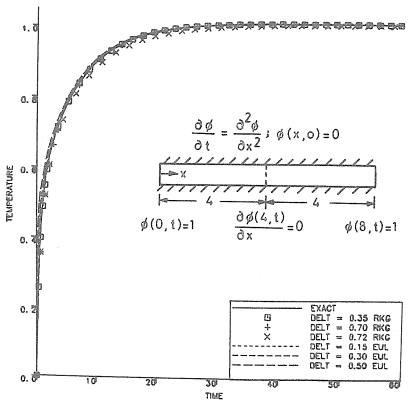

Fig. 1 - Temperature at x=1 by RKG scheme

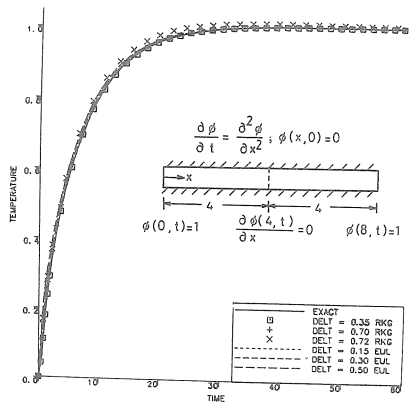

Fig. 2 - Temperature at x=2 by RKG scheme

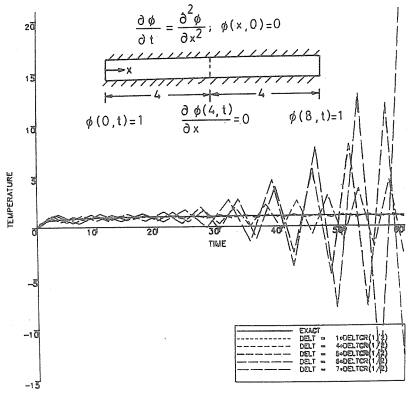

Fig. 3 - Temperature at x=1 by FEE scheme (θ = 1/2)

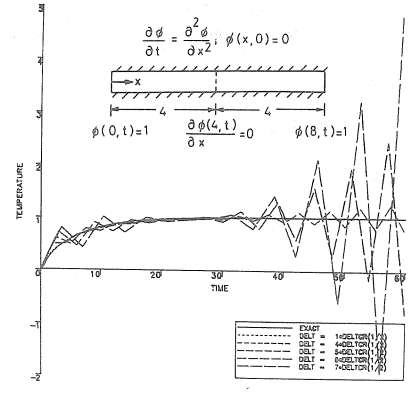

Fig. 4 - Temperature at x=2 by FEE scheme (θ = 1/2)

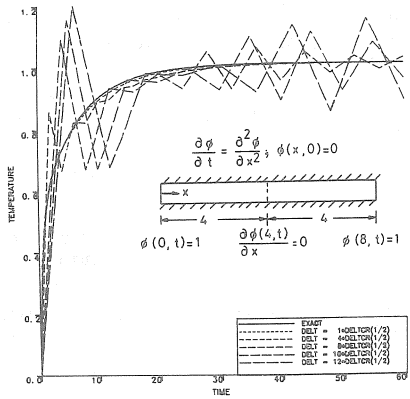

Fig. 5 - Temperature at x=1 by FEE scheme (θ = 2/3)

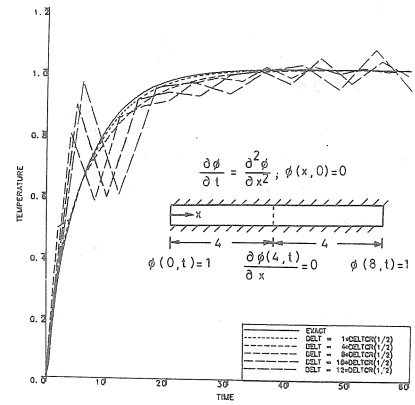

Fig. 6 - Temperature at x=2 by FEE scheme (θ = 2/3)

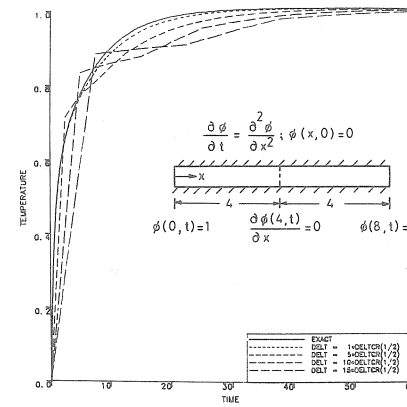

Fig. 7 - Temperature at x=1 by FEE scheme (θ = 1)

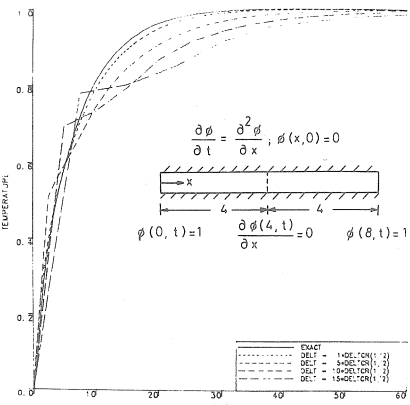

Fig. 8 - Temperature at x=2 by FEE scheme (θ = 1)