A Finite-Difference Method of High-Order Accuracy for the Solution of Three-Dimensional Transient Heat Conduction Problems

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A finite-difference method is presented for solving three-dimensional transient heat conduction problems. The method is a modification of the method of Douglas and Rachford which achieves the higher-order accuracy of a Crank-Nicholson formulation while preserving the advantages of the Douglas-Rachford method: unconditional stability and simplicity of solving the equations at each time level. Although the method has not yet been applied, the analysis in this paper suggests that it will prove to be the most efficient method yet proposed for the numerical integration of three-dimensional transient heat conduction problems.

Transient heat conduction problems in three dimensions represent a class of problems of great importance in many fields of engineering and science today. When the need for a numerical solution of such a problem arises, the requirements of computing time and of storage capacity often tax the capabilities of today's largest digital computers. Thus the need for more efficient finite-difference methods for solving such problems is an ever-constant one.

The differential equation describing transient heat conduction in an isotropic medium of constant thermal conductivity and volumetric heat capacity is

$$\frac{\partial^2 T}{\partial x^2}+\frac{\partial^2 T}{\partial y^2}+\frac{\partial^2 T}{\partial z^2}=\frac{\partial T}{\partial t} \tag{1}$$

where the time scale has been normalized to include the thermal diffusivity. Three well-known finite-difference approximations to Equation (1) are forward difference

$$\Delta^2_x(T_{i,j,k,n}) + \Delta^2_y(T_{i,j,k,n}) + \Delta^2_z(T_{i,j,k,n}) = \frac{(T_{i,j,k,n+1} - T_{i,j,k,n})}{\Delta t} \tag{2}$$

backward difference

$$\Delta^2_x(T_{i,j,k,n+1}) + \Delta^2_y(T_{i,j,k,n+1}) + \Delta^2_z(T_{i,j,k,n+1}) = \frac{(T_{i,j,k,n+1} - T_{i,j,k,n})}{\Delta t} \tag{3}$$

Crank-Nicholson (2)

$$\frac{\Delta^2_x(T_{i,j,k,n+1} + T_{i,j,k,n})}{2} + \frac{\Delta^2_y(T_{i,j,k,n+1} + T_{i,j,k,n})}{2} + \frac{\Delta^2_z(T_{i,j,k,n+1} + T_{i,j,k,n})}{2} = \frac{T_{i,j,k,n+1} - T_{i,j,k,n}}{\Delta t} \tag{4}$$

Equation (2) suffers from the stability limitation

$$\frac{\Delta t}{\Delta x^2}+\frac{\Delta t}{\Delta y^2}+\frac{\Delta t}{\Delta z^2} \leq \frac{1}{2} \tag{5}$$

Equations (3) and (4) are unconditionally stable. Equation (4) is of higher-order accuracy, thus permitting the use of larger values of Δt for a given desired accuracy. The use of Equation (3) or (4) relates the unknown temperatures at every point in the three-dimensional region by a system of simultaneous equations which must be solved for each time step. Although there are some very effective methods of iterating to the solution of these equations, this is nevertheless a formidable problem indeed. Douglas and Rachford (3) have developed an unconditionally stable finite-difference method with the accuracy of Equation (3) but with a greatly reduced amount of computation required for the solution at each time step. It is the purpose of this paper to present a modification of the Douglas-Rachford method which has the accuracy of Equation (4) but maintains unconditional stability and requires essentially the same computational effort at each time step as the method of Douglas and Rachford.

Consider the following finite-difference approximation to Equation (1):

$$\Delta^2_x(T^*_{i,j,k,n+1}) + \Delta^2_y(T_{i,j,k,n}) + \Delta^2_z(T_{i,j,k,n}) = \frac{(T^*_{i,j,k,n+1} - T_{i,j,k,n})}{\Delta t} \tag{6}$$

In Equation (6) the unknown values $T^*_{i,j,k,n+1}$ appear only in the time difference and in the x-direction difference. Thus only T^* values along a row parallel to the x-axis are related by a system of simultaneous equations. In contrast to the solution of Equations (3) and (4), Equation (6) requires the solution of many small, independent systems of simultaneous equations instead of one large system relating all T^* values within the three-dimensional region. Furthermore each system is tridiagonal, and a very efficient method for solving the tridiagonal system without iteration is well known (*1, 5, 6*).

If Equation (6) is used, and the T^* values are used as the temperatures at time level $n+1$, it is known that the stability limitation on this method is scarcely better than that shown in Equation (5). Thus T^* is considered as an intermediate approximation in the scheme, and Equation (6) is followed by

$$\Delta^2_x(T^*_{i,j,k,n+1}) + \Delta^2_y(T^{**}_{i,j,k,n+1}) + \Delta^2_z(T_{i,j,k,n}) = \frac{(T^{**}_{i,j,k,n+1} - T_{i,j,k,n})}{\Delta t} \tag{7}$$

$$\Delta^2_x(T^*_{i,j,k,n+1}) + \Delta^2_y(T^{**}_{i,j,k,n+1}) + \Delta^2_z(T^{***}_{i,j,k,n+1}) = \frac{(T^{***}_{i,j,k,n+1} - T_{i,j,k,n})}{\Delta t} \tag{8}$$

If the T^{***} values are taken to be the temperatures at the advanced time level $n+1$, the scheme of Equations (6), (7), and (8) is the unconditionally stable Douglas-Rachford method, although Douglas and Rachford presented their method in a slightly different form. The difference between Equations (7) and (6) is the second equation presented by Douglas and Rachford; the difference between Equations (8) and (7) is their third equation.

It is interesting to note that if the values T^{**} are used to evaluate the x-direction difference in Equation (8), the method of Equations (6), (7), and (8) is scarcely more stable than the forward finite-difference method of Equation (2). This is somewhat surprising because it might seem reasonable to assume that the most recently obtained approximation, T^{**}, should be used to evaluate both the x-direction and the y-direction differences in Equation (8). The fact that this is not the case is both interesting and somewhat baffling. A possible interpretation of this fact, which cannot be supported by rigorous argument but which may prove helpful in approaching similar stability problems in the future, is offered in the following discussion. It should be remembered that the T^{**} values are obtained by solution of Equation (7), and in this solution all values along a row parallel to the y axis are related by a system of simultaneous equations. Thus the T^{**} values are smoothed along rows parallel to the y axis and are thus highly suitable for use in the y-direction difference in Equation (8). If however the T^{**} values are used to evaluate the x-direction difference in Equation (8), this difference involves T^{**} values from different rows parallel to the y axis, and these values were in independent systems of simultaneous equations when the T^{**} values were computed. Thus the T^{**} values are not smoothed in the x direction, and it is imperative that they not be used in formulating the x-direction difference; the T^{*} values must be used for this purpose.

HIGHER-ORDER ACCURACY

The extension of these ideas to a system which is unconditionally stable but which has the accuracy of the Crank-Nicholson method, Equation (4), is the following proposed method:

$$\Delta^2_x(T^*_{i,j,k,n+1/2}) + \Delta^2_y(T_{i,j,k,n}) + \Delta^2_z(T_{i,j,k,n}) = \frac{(T^*_{i,j,k,n+1/2} - T_{i,j,k,n})}{(\Delta t/2)} \quad (9)$$

$$\Delta^2_x(T^*_{i,j,k,n+1/2}) + \Delta^2_y(T^{**}_{i,j,k,n+1/2}) + \Delta^2_z(T_{i,j,k,n}) = \frac{(T^{**}_{i,j,k,n+1/2} - T_{i,j,k,n})}{(\Delta t/2)} \quad (10)$$

$$\Delta^2_x(T^*_{i,j,k,n+1/2}) + \Delta^2_y(T^{**}_{i,j,k,n+1/2}) + \Delta^2_z(T^{***}_{i,j,k,n+1/2}) = \frac{(T^{***}_{i,j,k,n+1/2} - T_{i,j,k,n})}{(\Delta t/2)} \quad (11)$$

$$\Delta^2_x(T^*_{i,j,k,n+1/2}) + \Delta^2_y(T^{**}_{i,j,k,n+1/2}) + \Delta^2_z(T^{***}_{i,j,k,n+1/2}) = \frac{(T_{i,j,k,n+1} - T_{i,j,k,n})}{\Delta t} \quad (12)$$

The first three steps are seen to be equivalent to the Douglas-Rachford method for half of a time step. In the fourth step the temperatures at the advanced time level $n+1$ are computed explicitly with the distance differences formulated in terms of the T^*, T^{**}, and T^{***} values found in the first three steps. The form of this fourth step is similar to the Crank-Nicholson form, and the accuracy is approximately the same as that of Equation (4). For stability it is imperative that T^* be used for the x-direction differences, T^{**} be used for the y-direction differences, and T^{***} be used for the z-direction differences.

While Equations (9) through (12) present this new method in the manner best suited for conveying the ideas involved, computational ease and storage requirements suggest that a simpler form be used in practice:

$$\Delta^2_x(T^*_{i,j,k,n+1/2}) + \Delta^2_y(T_{i,j,k,n}) + \Delta^2_z(T_{i,j,k,n}) = \frac{(T^*_{i,j,k,n+1/2} - T_{i,j,k,n})}{(\Delta t/2)} \quad (9)$$

$$\Delta^2_y(T^{**}_{i,j,k,n+1/2}) - \Delta^2_y(T_{i,j,k,n}) = \frac{(T^{**}_{i,j,k,n+1/2} - T^*_{i,j,k,n+1/2})}{(\Delta t/2)} \quad (10a)$$

$$\Delta^2_z(T_{i,j,k,n+1}) - \Delta^2_z(T_{i,jk,n}) = \frac{(T_{i,j,k,n+1} + T_{i,j,k,n} - 2T^{**}_{i,j,k,n+1/2})}{(\Delta t/2)} \quad (11a)$$

Equation (10*a*) is the difference between Equations (10) and (9); Equation (11*a*) can be obtained by eliminating $T^{***}_{i,j,k,n+1/2}$ from the difference between Equations (11) and (10) by use of the difference between Equations (12) and (11).

Equation (9) relates the unknown T^* values along a row parallel to the x axis by a system of tridiagonal simultaneous equations, which can be solved without iteration (*1, 5, 6*). Such a system must be solved for each row parallel to the x axis. Equation (10*a*) is then solved in a similar manner, but this time the simultaneous equations relate T^{**} values along a row parallel to the y axis. The solution of Equation (11*a*) for the $T_{i,j,k,n+1}$ values is then accomplished in a similar manner with sets of tridiagonal simultaneous equations relating $T_{i,j,k,n+1}$ values along each row parallel to the z axis. The amount of computation required to solve these equations for each time level is approximately the same as that required in the Douglas-Rachford method. The amount of computation required is much less than that normally required to iterate to the solution of Equation (3) or (4); indeed it is only approximately four times that required to solve the explicit Equation (2).

COMPARISON WITH OTHER METHODS

Consider the problem of solving Equation (1) in a rectangular parallelepiped region

$$0 \leq x \leq 1,\ 0 \leq y \leq h,\ 0 \leq z \leq g \quad (13)$$

with the boundary conditions

$$\text{At } t = 0,\ T = \sin(\alpha\pi x)\sin(\beta\pi y/h)\sin(\gamma\pi z/g) \quad (14)$$

$$\text{For } t > 0,\ T = 0 \text{ on the boundaries of the region} \quad (15)$$

These boundary conditions are not as restrictive as they might at first appear. The initial condition, Equation (14), may be thought of as one term of a triple Fourier series representing an arbitrary initial temperature distribution. Likewise in any problem for which the temperature is specified, independent of time, along the boundaries of the region, a change of dependent variable to

$$T(x,y,z,t) - T_{\substack{\text{steady}\\ \text{state}}}(x,y,z)$$

will reduce the boundary conditions to the form of Equation (15).

For this problem the differential equation and the various finite-difference equations can be solved analytically. The solution to Equation (1) in the region (13), subject to the conditions (14) and (15), is

$$T(x,y,z,t) = [e^{-\pi^2(\alpha^2+\beta^2/h^2+\gamma^2/g^2)t}]\sin(\alpha\pi x)\sin(\beta\pi y/h)\sin(\gamma\pi z/g) \quad (16)$$

The solutions to the various finite-difference equations to be considered can be put into a common form

$$T_{i,j,k,n} = (\xi)^n \sin(\alpha\pi i\Delta x)\sin(\beta\pi j\Delta y/h)\sin(\gamma\pi k\Delta z/g) \quad (17)$$

TABLE 1. COMPARISON OF DECAY FACTORS FOR Δx, Δy, $\Delta z \to 0$

	Decay factors				
$\pi^2\left(\alpha^2+\frac{\beta^2}{h^2}+\frac{\gamma^2}{g^2}\right)\Delta t$	Differential equation, ξ_T	Equation (3), ξ°_B	Equation (4), ξ°_{CN}	Douglas-Rachford*, ξ°_{DR}	Proposed new method*, ξ°_P
0.01	0.9900498	0.9900990	0.9900498	0.9900993	0.9900498
0.04	0.9607894	0.9615385	0.9607843	0.9615583	0.9607895
0.05	0.9512294	0.9523810	0.9512195	0.9524189	0.9512295
0.10	0.9048374	0.9090909	0.9047619	0.9093686	0.9048378
0.20	0.8187308	0.8333333	0.8181818	0.8352051	0.8187348
0.40	0.6703200	0.7142857	0.6666667	0.7213910	0.6704101
0.50	0.6065307	0.6666667	0.6000000	0.6851312	0.6067365
1.0	0.3678794	0.5000000	0.3333333	0.5781250	0.3702624
2.0	0.1353353	0.3333333	0.0000000	0.5680000	0.1562500

* ξ°_{DR} and ξ°_P values reported are for $\alpha = \beta/h = \gamma/g$.

where for the forward difference Equation (2)

$$\xi_F = 1 - X - Y - Z$$

For the backward difference Equation (3)

$$\xi_B = 1/(1 + X + Y + Z)$$

For the Crank-Nicholson Equation (4)

$$\xi_{CN} = \frac{1 - \frac{1}{2}(X+Y+Z)}{1 + \frac{1}{2}(X+Y+Z)}$$

For the Douglas-Rachford method, Equations (6), (7), and (8)

$$\xi_{DR} = \frac{1 + (XY + XZ + YZ + XYZ)}{1 + X + Y + Z + (XY + XZ + YZ + XYZ)}$$

and for the proposed new method Equations (9), (10*a*), and (11*a*)

$$\xi_P = \frac{1 - \frac{1}{2}(X+Y+Z) + \frac{1}{4}(XY + XZ + YZ + \frac{1}{2}XYZ)}{1 + \frac{1}{2}(X+Y+Z) + \frac{1}{4}(XY + XZ + YZ + \frac{1}{2}XYZ)}$$

By comparing Equations (16) and (17) it is clear that the accuracy of each finite-difference method, for this simple problem, can be assessed by comparing its decay factor with the decay factor in the true solution to the differential equation:

$$\xi_T = e^{-\pi^2(\alpha^2+\beta^2/h^2+\gamma^2/g^2)\Delta t}$$

It is also clear that if inequality (5) is violated, $|\xi_F|$ will exceed unity for certain frequencies α, β, and γ, and thus the forward difference Equation (2) will be unstable. The other finite difference methods are unconditionally stable, $|\xi|$ remaining less than unity for all positive values of X, Y, and Z.

It is instructive to compare the solutions of these various methods for the problem outlined. In the limiting case

$$\Delta x \to 0,\ \Delta y \to 0,\ \Delta z \to 0$$

it can be seen that

$$X \to (\alpha\pi)^2\Delta t$$
$$Y \to (\beta\pi/h)^2\Delta t$$
$$Z \to (\gamma\pi/g)^2\Delta t$$

and the decay factors ξ° can be computed readily. These decay factors are compared in Table 1 for various values of the time increment Δt. The value of ξ°_P depends on the ratios of α, β/h, and γ/g. If two of these three frequencies are zero, then

$$\xi^\circ_P = \xi^\circ_{CN}$$

If on the other hand

$$\alpha = \beta/h = \gamma/g \qquad (18)$$

then ξ°_P shows a maximum deviation from ξ°_{CN}. The value of ξ°_P will always lie between these two extremes. The values of ξ°_P reported in Table 1 were computed with Equation (18) assumed to be true. Thus for example at

$$\pi^2(\alpha^2 + \beta^2/h^2 + \gamma^2/g^2)\Delta t = 0.2$$

the value of ξ°_P will always lie between 0.8187348 and 0.8181818, depending upon the relative values of α, β/h, and γ/g. Similarly ξ°_{DR} will always lie between 0.8352051 and 0.8333333, which is the reported value of ξ°_B.

It is clear, from Table 1, that the proposed new method and Equation (4) are considerably more accurate than the Douglas- Rachford method and Equation (3). For example at a value of

$$t = 2/\pi^2(\alpha^2 + \beta^2/h^2 + \gamma^2/g^2)$$

the true solution to the differential equation is

$$T = (e^{-2})\sin(\alpha\pi x)\sin(\beta\pi y/h)\sin(\gamma\pi z/g) = (0.1353)\sin(\alpha\pi x)\sin(\beta\pi y/h)\sin(\gamma\pi z/g)$$

If

$$\Delta t = 0.2/\pi^2(\alpha^2 + \beta^2/h^2 + \gamma^2/g^2)$$

the solution given by the proposed new method will be between

$$(0.8187348)^{10} \text{ and } (0.8181818)^{10}$$

times the three sine terms, or between

$$(0.1353)\sin(\alpha\pi i\Delta x)\sin(\beta\pi j\Delta y/h)\sin(\gamma\pi k\Delta z/g)$$

and

$$(0.1344)\sin(\alpha\pi i\Delta x)\sin(\beta\pi j\Delta y/g)\sin(\gamma\pi k\Delta z/g)$$

depending upon the relative values of α, β/h, and γ/g. Thus the error in this method is less than 1%. If the Douglas-Rachford method were used with the same value of Δt, the solution would be between

$$(0.8352051)^{10} \text{ and } (0.8333333)^{10}$$

times the three sine terms, or between

$$(0.1653)\sin(\alpha\pi i\Delta x)\sin(\beta\pi j\Delta y/h)\sin(\gamma\pi k\Delta z/g)$$

and

$$(0.1615)\sin(\alpha\pi i\Delta x)\sin(\beta\pi j\Delta y/h)\sin(\gamma\pi k\Delta z/g)$$

which is 19 to 22% higher than the solution to the differential equation. Indeed if

$$\Delta t = 0.01/\pi^2(\alpha^2 + \beta^2/h^2 + \gamma^2/g^2)$$

the solution to the Douglas-Rachford method is

$$(0.990099)^{200}$$

times the three sine terms, or

$$(0.1365)\sin(\alpha\pi i\Delta x)\sin(\beta\pi j\Delta y/h)\sin(\gamma\pi k\Delta z/g)$$

which is the same degree of accuracy that the new method obtained with a value of Δt twenty times as large.

If the new method is used with

$$\Delta t = 0.4/\pi^2(\alpha^2 + \beta^2/h^2 + \gamma^2/g^2)$$

the result will be approximately 3% too low at

$$t = 2/\pi^2(\alpha^2 + \beta^2/h^2 + \gamma^2/g^2)$$

The Rachford-Douglas method requires one-tenth this value of Δt to achieve an accuracy of 3%.

Other comparisons with the values in Table 1 and also comparisons with values of Δx, Δy, and Δz greater than zero yield the same conclusion: the proposed new method is of the same order of accuracy as Equation (4), and this is a substantial improvement over the Douglas-Rachford method and Equation (3). It would be expected that this conclusion would hold true for other problems with more complicated boundary conditions, but this has not yet been demonstrated.

NONLINEAR PROBLEMS

If Equation (1) were modified to contain a nonlinear heat source or heat sink term, the proposed method would appear to be well suited to this modification. In this case the four-step form would probably be preferable to the three-step form. Equations (9), (10), and (11) could be used with the nonlinear term evaluated at the temperatures at the present time level n, and then Equation (12) could be used with the nonlinear term evaluated at the values $T^{***}_{i,j,k,n+1/2}$. This formulation would allow a high-order accuracy approximation to the nonlinear term in the final step, and it is analogous to the method proposed by Douglas (4) for obtaining high-order accuracy in such nonlinear terms. Such a procedure is not advisable however in the case where Equation (1) is modified by a nonlinear coefficient multiplying the time derivative (or the distance derivatives). For example if Equations (9), (10), and (11) were used with the coefficient evaluated in terms of temperatures at time level n, and then Equation (12) were used with the coefficient evaluated in terms of the T^{***} values, a stability limitation would result if the coefficient multiplying the time derivative were smaller in the fourth step than in the first three steps. This would be similar to a linear problem in which the time increment for the fourth step was larger than twice the time increment for the first three steps. A better procedure for obtaining an accurate approximation to the nonlinear coefficient might be to use an equation such as Equation (9), with the coefficient evaluated from temperatures at time level n to get an approximation to the $n+\frac{1}{2}$ level temperatures. These temperatures could then be used to evaluate the coefficient for the entire computation of Equations (9), (10), (11), and (12), or Equations (9), (10*a*), and (11*a*). A conclusion as to the suitability of this method for nonlinear problems will of course have to await the use of the method in some test problems.

TWO-DIMENSIONAL PROBLEMS

For two-dimensional heat conduction this new method is identical to the alternating-direction implicit method of Peaceman and Rachford (5). For a two-dimensional problem with a nonlinear heat source or heat sink term it is likely that a three-step formulation analogous to Equations (9), (10), (11), and (12) would be preferable to the two-step formulation presented by Peaceman and Rachford because it would permit the evaluation of the nonlinear term at the half-time level for the final step, as discussed in the preceding paragraph.

CONCLUSION

A new finite-difference method has been proposed for solving three-dimensional transient heat conduction problems, and this method has been shown to be unconditionally stable for linear problems. The computing time required to solve the equations at each time step is approximately the same as that required by the highly efficient method of Douglas and Rachford, but the new method has the higher-order accuracy of a Crank-Nicholson method, and so the time increment can be chosen larger than in the Douglas-Rachford method. A simple example problem, for which the finite-difference equations could be solved analytically, was offered to show that the magnitude of the allowable increase in the time increment could be of the order of a factor of 10 or 20.

It should be emphasized that this proposed method has not yet been applied, and the ultimate evaluation of the method must await application. Nevertheless the considerations presented in this paper lead the author to anticipate that the new method will prove to be the most efficient method yet proposed for the numerical solution of three-dimensional transient heat conduction problems.

NOTATION

e = 2.71828 . . .

g = length of rectangular parallelepiped region in z direction

h = length of rectangular parallelepiped region in y direction

i = $x/\Delta x$, an integer

j = $y/\Delta y$, an integer

k = $z/\Delta z$, an integer

n = $t/\Delta t$, an integer

T = temperature

$T_{i,j,k,n}$ = $T(i\Delta x,\ j\Delta y,\ k\Delta z,\ n\Delta t)$

$\Delta^2_x(T_{i,j,k,n}) = \dfrac{T_{i-1,j,k,n} - 2T_{i,j,k,n} + T_{i+1,j,k,n}}{\Delta x^2}$, the second difference in the x direction, analogous definitions for y and z directions

t = time, in units chosen to normalize the thermal diffusivity

x = distance in the x direction

X = $4\dfrac{\Delta t}{\Delta x^2}\sin^2\left(\dfrac{\alpha\pi\Delta x}{2}\right)$

Δx = increment in x

y = distance in the y direction

Y = $4\dfrac{\Delta t}{\Delta y^2}\sin^2\left(\dfrac{\beta\pi\Delta y}{2h}\right)$

Δy = increment in y

z = distance in the z direction

Z = $4\dfrac{\Delta t}{\Delta z^2}\sin^2\left(\dfrac{\gamma\pi\Delta z}{2g}\right)$

Δz = increment in z

Greek Letters

α = frequency of sinusoidal variation in x direction, an integer

β = frequency of sinusoidal variation in y direction, an integer

γ = frequency of sinusoidal variation in z direction, an integer

ξ = decay factor

π = 3.14159 . . .

Subscripts

B = backward difference method

CN = Crank-Nicholson method

DR = Douglas-Rachford method

F = forward difference method

P = proposed new method

T = true solution to the differential equation

Superscripts

$*$, $**$, $***$ = intermediate values used for x-, y-, and z-direction differences, respectively

o = limiting value as Δx, Δy, $\Delta z \rightarrow o$

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