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SOL: AN ORACLE CODE FOR THE
SOLUTION OF CERTAIN SECOND ORDER
LINEAR PARTIAL DIFFERENTIAL EQUATIONS

OAK RIDGE NATIONAL LABORATORY

operated by

UNION CARBIDE CORPORATION

for the

U.S. ATOMIC ENERGY COMMISSION

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**SOL: AN ORACLE CODE FOR THE SOLUTION OF
CERTAIN SECOND ORDER LINEAR PARTIAL DIFFERENTIAL EQUATIONS**

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Oak Ridge, Tennessee
operated by
UNION CARBIDE CORPORATION
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U.S. ATOMIC ENERGY COMMISSION

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ABSTRACT

This report describes in detail the numerical solution of a second-order linear partial differential equation of the form

$$\frac{\partial \eta(x,t)}{\partial t} = A(x) \frac{\partial^2 \eta(x,t)}{\partial x^2} + \left[\frac{g}{x} + B(x) \right] \frac{\partial \eta(x,t)}{\partial x} + C(x) \eta(x,t) + D(x,t)$$

with two-point boundary conditions and zero initial condition.

An Oracle code is described which solves this equation for $D(x,t) = D(x)$, and it is shown that this code may be used to solve the differential equation $A(x) \eta'' + B(x) \eta' + C(x) \eta + D(x) = 0$ with two point boundary conditions.

1. INTRODUCTION

SOL is an Oracle code for the solution of the second-order linear partial differential equation of the form:

$$\frac{\partial \eta(x,t)}{\partial t} = A(x) \frac{\partial^2 \eta(x,t)}{\partial x^2} + \left[\frac{g}{x} + B(x) \right] \frac{\partial \eta(x,t)}{\partial x} + C(x) \eta(x,t) + D(x) \quad (1)$$

with boundary conditions

$$M_0 \frac{\partial \eta(x_0,t)}{\partial x} + N_0 \eta(x_0,t) + L_0 = 0 \quad (2a)$$

$$M_N \frac{\partial \eta(x_{n-1},t)}{\partial x} + N_N \eta(x_{n-1},t) + L_N = 0 \quad (N = n - 1) , \quad (2b)$$

and the initial condition $\eta(x,0) = 0$. The code is so written that various deviations from Eq. (1) may be solved by simply rewriting certain items and recompiling the corresponding section of the code. In reactor analysis SOL may be interpreted as a multiregion, one-group, time-dependent code. On page 11 it is shown how, without any changes in the code, a second-order linear ordinary differential equation may be solved.

The author is indebted to R. R. Coveyou, whose advice was sought on several occasions with regard to the analysis of this report.

2. ANALYSIS

Equations similar to (1) occur when D is a function of both x and t . The following analysis is for that case; however, the Oracle code was written for D as a function of x only.

The difference equation for (1) as a function of t is as follows:

$$\begin{aligned} \frac{\eta(x, t + \Delta t) - \eta(x, t)}{\Delta t} = & P \left\{ A(x) \frac{\partial^2 \eta(x, t + \Delta t)}{\partial x^2} + \left[\frac{g}{x} + B(x) \right] \frac{\partial \eta(x, t + \Delta t)}{\partial x} + \right. \\ & \left. + C(x) \eta(x, t + \Delta t) + D(x, t + \Delta t) \right\} + Q \left\{ A(x) \frac{\partial^2 \eta(x, t)}{\partial x^2} + \left[\frac{g}{x} + B(x) \right] \frac{\partial \eta(x, t)}{\partial x} + \right. \\ & \left. + C(x) \eta(x, t) + D(x, t) \right\} + R \left\{ A(x) \frac{\partial^2 \eta(x, t - \Delta t)}{\partial x^2} + \left[\frac{g}{x} + B(x) \right] \frac{\partial \eta(x, t - \Delta t)}{\partial x} + \right. \\ & \left. + C(x) \eta(x, t - \Delta t) + D(x, t - \Delta t) \right\} , \end{aligned} \quad (3)$$

where P , Q , and R are constants which satisfy certain accuracy and validity conditions as set forth on pages 7-9.

By combining terms in Eq. (3) and dividing by $P A(x)$, the resulting expression reduces to the second-order differential equation

$$\frac{\partial^2 \eta(x, t + \Delta t)}{\partial x^2} + A_1(x) \frac{\partial \eta(x, t + \Delta t)}{\partial x} + B_1(x) \eta(x, t + \Delta t) + C_1(x, t + \Delta t) = 0 , \quad (4)$$

where

$$\begin{aligned} A_1(x) &= \frac{(g/x) + B(x)}{A(x)} , \\ B_1(x) &= \frac{P C(x) - (1/\Delta t)}{P A(x)} , \\ C_1(x, t + \Delta t) &= \frac{1}{P} \left\{ Q \frac{\partial^2 \eta(x, t)}{\partial x^2} + R \frac{\partial^2 \eta(x, t - \Delta t)}{\partial x^2} + \right. \\ &+ A_1(x) \left[Q \frac{\partial \eta(x, t)}{\partial x} + R \frac{\partial \eta(x, t - \Delta t)}{\partial x} \right] + \frac{Q C(x) + (1/\Delta t)}{A(x)} \eta(x, t) + \frac{R C(x)}{A(x)} \eta(x, t - \Delta t) + \\ &\left. + \frac{P D(x, t + \Delta t) + Q D(x, t) + R D(x, t - \Delta t)}{A(x)} \right\} . \end{aligned} \quad (5)$$

The computation of $C_1(x, t + \Delta t)$ involves an iterative process; therefore, a detailed discussion concerning the evaluation of this function is given later.

To set up the iteration for the solution at $t = \Delta t$, it is assumed that $P = Q = \frac{1}{2}$ and $R = 0$.
For this case

$$\begin{aligned} A_1(x) &= \frac{(g/x) + B(x)}{A(x)}, \\ B_1(x) &= \frac{C(x) - (2/\Delta t)}{A(x)}, \\ C_1(x, \Delta t) &= \frac{D(x, \Delta t) + D(x, 0)}{A(x)}, \end{aligned} \quad (6)$$

where x is given by

$$x = x_0 + ib,$$

in which

x_0 = the initial value of x ,

i = an integer,

b = the increment in x .

The solution of Eq. (4) is accomplished by using central difference formulas accurate to a fourth-order correction factor. Since only the solution of an ordinary differential equation is being considered here, $\eta(x, t)$ will be replaced by $\eta(x)$, and $d\eta(x)/dx$ will be replaced by $\eta^i(x)$.

If

$$\frac{\eta(x+b) - \eta(x-b)}{2b}$$

is expanded in a Taylor series about x , then

$$\eta^i(x) \cong \frac{\eta(x+b) - \eta(x-b)}{2b} - \frac{b^2 \eta^{iii}(x)}{6} + \dots + O(b^4), \quad (7)$$

where $O(b^4)$ signifies a correction term in which b^4 is a factor. If

$$\frac{\eta(x+b) - 2\eta(x) + \eta(x-b)}{b^2}$$

is expanded as above, then

$$\eta^{ii}(x) \cong \frac{\eta(x+b) - 2\eta(x) + \eta(x-b)}{b^2} - \frac{b^2 \eta^{iv}(x)}{12} + \dots + O(b^4). \quad (8)$$

From Eq. (4),

$$\eta^{ii}(x) = -[A_1(x) \eta^i(x) + B_1(x) \eta(x) + C_1(x)],$$

$$\eta^{iii}(x) = -\left\{A_1(x) \eta^{ii}(x) + [A_1^i(x) + B_1(x)] \eta^i(x) + B_1^i(x) \eta(x) + C_1^i(x)\right\}, \quad (9)$$

and

$$\eta^{iv}(x) = - \left\{ A_1(x) \eta^{iii}(x) + [2A_1^i(x) + B_1(x)] \eta^{ii}(x) + [A_1^{ii}(x) + 2B_1^i(x)] \eta^i(x) + B_1^{ii}(x) \eta(x) + C_1^{ii}(x) \right\} .$$

By substituting for $\eta^{iii}(x)$,

$$\begin{aligned} \eta^{iv}(x) = & [A_1^2(x) - 2A_1^i(x) - B_1(x)] \eta^{ii}(x) + [A_1(x) A_1^i(x) + \\ & + A_1(x) B_1(x) - A_1^{ii}(x) - 2B_1^i(x)] \eta^i(x) + [A_1(x) B_1^i(x) - B_1^{ii}(x)] \eta(x) + \\ & + [A_1(x) C_1^i(x) - C_1^{ii}(x)] . \end{aligned} \quad (10)$$

Only a second-order correction term is required for Eqs. (9) and (10); hence

$$\eta^i(x) = \frac{\eta(x+b) - \eta(x-b)}{2b}$$

and

$$\eta^{ii}(x) = \frac{\eta(x+b) - 2\eta(x) + \eta(x-b)}{b^2}$$

may be substituted directly into these equations. Therefore,

$$\eta^{iii}(x) = - \frac{A_2(x) \eta(x+b) + B_2(x) \eta(x) + C_2(x) \eta(x-b) + H_2(x)}{2b^2} \quad (11)$$

and

$$\eta^{iv}(x) = \frac{D_2(x) \eta(x+b) + E_2(x) \eta(x) + F_2(x) \eta(x-b) + G_2(x)}{2b^2} , \quad (12)$$

where

$$A_2(x) = 2A_1(x) + [A_1^i(x) + B_1(x)] b ,$$

$$B_2(x) = 2[B_1^i(x) b^2 - 2A_1(x)] ,$$

$$C_2(x) = 2A_1(x) - [A_1^i(x) + B_1(x)] b ,$$

$$D_2(x) = 2[A_1^2(x) - 2A_1^i(x) - B_1(x)] + \left\{ A_1(x) [A_1^i(x) + B_1(x)] - A_1^{ii}(x) - 2B_1^i(x) \right\} b ,$$

$$E_2(x) = 4[B_1(x) + 2A_1^i(x) - A_1^2(x)] + 2[A_1(x) B_1^i(x) - B_1^{ii}(x)] b^2 ,$$

$$F_2(x) = 2[A_1^2(x) - 2A_1^i(x) - B_1(x)] - \left\{ A_1(x) [A_1^i(x) + B_1(x)] - A_1^{ii}(x) - 2B_1^i(x) \right\} b ,$$

$$G_2(x) = 2[A_1(x) C_1^i(x) - C_1^{ii}(x)] b^2 ,$$

$$H_2(x) = 2C_1^i(x) b^2 .$$

If Eqs. (7), (8), (11), and (12) are substituted into Eq. (4) and the resulting expression is multiplied by $b^2/2$, then

$$\begin{aligned} & \left[\frac{1}{2} - \frac{D_2(x) b^2}{48} + \frac{A_1(x) b}{4} + \frac{A_1(x) A_2(x) b^2}{24} \right] \eta(x+b) - \left[1 + \frac{E_2(x) b^2}{48} - \right. \\ & \quad \left. - \frac{A_1(x) B_2(x) b^2}{24} - \frac{B_1(x) b^2}{2} \right] \eta(x) + \left[\frac{1}{2} - \frac{F_2(x) b^2}{48} + \frac{A_1(x) C_2(x) b^2}{24} - \right. \\ & \quad \left. - \frac{A_1(x) b}{4} \right] \eta(x-b) + \left[\frac{A_1(x) H_2(x) b^2}{24} - \frac{G_2(x) b^2}{48} + \frac{C_1(x) b^2}{2} \right] = 0 . \quad (13) \end{aligned}$$

Equation (13) is divided by the coefficient of $\eta(x)$, and $\eta(x+b)$ is replaced by T_{k+1} to give

$$P_k T_{k+1} - T_k + R_k T_{k-1} + S_k = 0 , \quad (14)$$

where

$$P_k = \left[\frac{1}{2} - \frac{D_2(x) b^2}{48} + \frac{A_1(x) b}{4} + \frac{A_1(x) A_2(x) b^2}{24} \right] / Q_k ,$$

$$R_k = \left[\frac{1}{2} - \frac{F_2(x) b^2}{48} + \frac{A_1(x) C_2(x) b^2}{24} - \frac{A_1(x) b}{4} \right] / Q_k ,$$

$$S_k = \left[\frac{A_1(x) H_2(x) b^2}{24} - \frac{G_2(x) b^2}{48} + \frac{C_1(x) b^2}{2} \right] / Q_k ,$$

$$Q_k = \left[1 + \frac{E_2(x) b^2}{48} - \frac{A_1(x) B_2(x) b^2}{24} - \frac{B_1(x) b^2}{2} \right] .$$

If

$$T_{k-1} = \Gamma_{k-1} T_k + \Delta_{k-1} , \quad (15)$$

then, since Eq. (14) reduces to

$$T_k = \frac{P_k}{1 - R_k \Gamma_{k-1}} T_{k+1} + \frac{R_k \Delta_{k-1} + S_k}{1 - R_k \Gamma_{k-1}} , \quad (16)$$

it follows that

$$\Gamma_k = \frac{P_k}{1 - R_k \Gamma_{k-1}} \quad (17)$$

and

$$\Delta_k = \frac{R_k \Delta_{k-1} + S_k}{1 - R_k \Gamma_{k-1}}. \quad (18)$$

Recursion formulas (17), (18), and (15) may be solved if Γ_0 , Δ_0 , and T_{n-1} are known. The values of these quantities are given below.

The boundary conditions are of the form

$$M_j \eta^i + N_j \eta + L_j = 0 \quad (j = 0, j = N). \quad (19)$$

The difference equation of (19) is

$$D_j \eta(x+b) + E_j \eta(x) + F_j \eta(x-b) + G_j = 0, \quad (20)$$

where

$$D_j = M_j [6 + A_{2j}(x) b],$$

$$E_j = [M_j B_{2j}(x) + 12N_j] b,$$

$$F_j = M_j [C_{2j}(x) b - 6],$$

and

$$G_j = [M_j H_{2j}(x) + 12L_j] b.$$

Here $A_{2j}(x) = A_2(x + jb)$, etc.

If $M_0 \neq 0$, then Γ_0 and Δ_0 may be found by eliminating T_{-1} from Eqs. (14) and (20), where $k = j = 0$. This gives

$$T_0 = \frac{F_0 P_0 - D_0 R_0}{E_0 R_0 + F_0} T_1 + \frac{F_0 S_0 - G_0 R_0}{E_0 R_0 + F_0}.$$

Thus for $M_0 \neq 0$,

$$\Gamma_0 = \frac{F_0 P_0 - D_0 R_0}{E_0 R_0 + F_0}, \quad (21a)$$

$$\Delta_0 = \frac{F_0 S_0 - G_0 R_0}{E_0 R_0 + F_0}. \quad (21b)$$

If $M_0 = 0$, then

$$\eta(x) = \frac{-L_0}{N_0}.$$

From Eq. (15) this gives

$$\Gamma_0 = 0 , \quad (22a)$$

$$\Delta_0 = \frac{-L_0}{N_0} . \quad (22b)$$

If $M_N \neq 0$,

$$D_N T_{N+1} + E_N T_N + F_N T_{N-1} + G_N = 0 . \quad (23)$$

Upon solving Eqs. (14), (15), and (23) for T_N , where $k = N$,

$$T_N = \frac{H_N \Delta_N - J_N \Gamma_N}{H_N - \Gamma_N I_N} , \quad (24)$$

where

$$H_N = F_N P_N - D_N R_N ,$$

$$I_N = F_N + E_N R_N ,$$

$$J_N = F_N S_N - G_N R_N .$$

If $M_N = 0$,

$$T_N = \frac{-L_N}{N_N} . \quad (25)$$

Of prime importance is the accuracy and validity of the approximation using the forward difference approximation for the t -derivative.

In the following, it is assumed that for each term of the solution the variables may be separated. Since only one such term will then need to be considered, $\eta(x, t)$ will be assumed to be of this form.

Thus

$$\eta(x, t) = \eta(x) T(t) . \quad (26)$$

Also

$$\frac{\partial^n \eta(x, t)}{\partial x^n} = T(t) \frac{d^n \eta(x)}{dx^n}$$

and

$$\frac{\partial \eta(x, t)}{\partial t} = \eta(x) \frac{dT(t)}{dt} .$$

It will also be assumed that $D(x, t)$ is of the form $T(t) P(x)$.

If L is the operator

$$L[\eta(x)] = A(x) \frac{d^2 \eta(x)}{dx^2} + \left[\frac{g}{x} + B(x) \right] \frac{d\eta(x)}{dx} + C(x) \eta(x) + P(x) ,$$

then Eq. (3) becomes, as $\Delta t \rightarrow 0$,

$$\eta(x) \frac{dT(t)}{dt} = P T(t + \Delta t) L[\eta(x)] + Q T(t) L[\eta(x)] + R T(t - \Delta t) L[\eta(x)] . \quad (27)$$

The variables of Eq. (27) may be separated; thus, introducing a parameter, λ ,

$$\frac{1}{P T(t + \Delta t) + Q T(t) + R T(t - \Delta t)} \frac{dT(t)}{dt} = \lambda , \quad (28)$$

$$\frac{L[\eta(x)]}{\eta(x)} = \lambda .$$

Since Eq. (28) holds for small Δt , and from Eq. (3), $(P + Q + R) \rightarrow 1$ as $\Delta t \rightarrow 0$, the solution of Eq. (28) for Δt small is assumed to be of the form

$$T(t) = ae^{\lambda t} . \quad (29)$$

Using forward difference approximation, Eq. (28) becomes

$$\frac{T(t + \Delta t) - T(t)}{\Delta t [P T(t + \Delta t) + Q T(t) + R T(t - \Delta t)]} = \lambda , \quad (30)$$

which simplifies to

$$(1 - \lambda P \Delta t) T(t + \Delta t) - (1 + \lambda Q \Delta t) T(t) - \lambda R \Delta t T(t - \Delta t) = 0 . \quad (31)$$

If $T(t) = T(n \Delta t) = w^n$, Eq. (31) reduces to

$$(1 - \lambda P \Delta t) w^2 - (1 + \lambda Q \Delta t) w - \lambda R \Delta t = 0 . \quad (32)$$

If w_1 and w_2 are the roots of Eq. (32) and w_1 approximates $e^{\lambda \Delta t}$, the general solution for $T(t)$ is

$$T(n \Delta t) = a w_1^n + b w_2^n$$

or

$$\frac{T(n \Delta t)}{w_1^n} = a + b \left(\frac{w_2}{w_1} \right)^n ,$$

which satisfies Eq. (29) if

$$\left(\frac{w_2}{w_1} \right)^n \approx 0 .$$

Hence the choice of P , Q , and R will be based upon the following criteria:

A. The root of Eq. (32) which is larger in absolute value should approximate $e^{\lambda \Delta t}$ for λ small.

B. The absolute value of the root of interest should be large in comparison with the absolute value of the other root.

The choice of P , Q , and R for accuracy may be established in the following manner. If $W = e^{\lambda \Delta t}$, then by expanding $e^{\lambda \Delta t}$ and $e^{2\lambda \Delta t}$ in a Taylor series about 0 and dropping terms containing $(\Delta t)^4$, Eq. (32) becomes

$$\lambda \Delta t (1 - P - Q - R) + (\lambda \Delta t)^2 \left(\frac{3}{2} - 2P - Q \right) + (\lambda \Delta t)^3 \left(\frac{7}{6} - 2P - \frac{Q}{2} \right) = 0 .$$

Therefore for fourth-order accuracy in Δt ,

$$P + Q + R = 1 , \quad (33a)$$

$$4P + 2Q = 3 , \quad (33b)$$

$$12P + 3Q = 7 . \quad (33c)$$

The solution of this system of equations is

$$P = \frac{5}{12} , \quad Q = \frac{2}{3} , \quad R = \frac{-1}{12} .$$

However, these values may not satisfy conditions A and B, in which case the approximation will not be valid.

If Eqs. (33a) and (33b) are taken as a minimum accuracy condition, the following may be said:

1. The initial values, $P = Q = \frac{1}{2}$, $R = 0$, guarantee that conditions A and B are satisfied.
2. If, for another set of values of P , Q , and R , better satisfying Eqs. (33a), (33b), and (33c), the solution converges in t to the solution given by $P = Q = \frac{1}{2}$, $R = 0$, then there is an $n \Delta t$ at which a more accurate solution is obtained by using the new set.

Generally, each problem must be considered on its own merit if values for P , Q , and R different from the initial values are desired. Further discussion of this is given in Sec. 4.

The only coefficient of Eq. (4) which is time-dependent is $C_1(x, t + \Delta t)$; hence considerable attention must be given to the computation of this function.

Letting

$$W(x, t) = \eta''(x, t) + A_1(x) \eta'(x, t) + \frac{C(x)}{A(x)} \eta(x, t) + \frac{D(x, t)}{A(x)} ,$$

then from Eq. (5),

$$C_1(x, t + \Delta t) = \frac{Q}{P} W(x, t) + \frac{R}{P} W(x, t - \Delta t) + \frac{D(x, t + \Delta t)}{A(x)} + \frac{1}{P \Delta t A(x)} \eta(x, t) . \quad (34)$$

From Eqs. (7), (8), (9), and (10)

$$W(x, t) = \alpha \eta(x + b, t) + \beta \eta(x, t) + \gamma \eta(x - b, t) + \delta(x, t) + \frac{D(x, t)}{A(x)} , \quad (35)$$

where

$$\alpha = \left[\frac{1}{b^2} - \frac{D_2(x)}{24} \right] + \left[\frac{1}{2b} + \frac{A_2(x)}{12} \right] A_1(x) ,$$

$$\beta = \frac{A_1(x) B_2(x)}{12} + \frac{C(x)}{A(x)} - \frac{2}{b^2} - \frac{E_2(x)}{24} ,$$

$$\gamma = \left[\frac{1}{b^2} - \frac{F_2(x)}{24} \right] + \left[\frac{C_2(x)}{12} - \frac{1}{2b} \right] A_1(x) ,$$

$$\delta(x,t) = \left[\frac{A_1(x) b + 2}{24} \right] C_1(x+b,t) - \frac{1}{6} C_1(x,t) + \left[\frac{2 - A_1(x) b}{24} \right] C_1(x-b,t) .$$

Thus

$$C_1(x,t + \Delta t) = \frac{\alpha}{P} f(x+b,t) + \frac{\beta}{P} f(x,t) + \frac{\gamma}{P} f(x-b,t) + \theta ,$$

where

$$f(x,t) = Q \eta(x,t) + R \eta(x,t - \Delta t) ,$$

$$\theta = \left\{ A(x) [Q \delta(x,t) + R \delta(x,t - \Delta t)] + \frac{1}{\Delta t} \eta(x,t) + P D(x,t + \Delta t) + Q D(x,t) + R D(x,t - \Delta t) \right\} / P A(x) .$$

Although SOL was not written to solve a second-order linear ordinary differential equation with a two-point boundary condition, such an equation may be solved by simply varying the input as indicated in Sec. 3.

3. THE ORACLE CODE

In SOL it is assumed that all the input information is stored on drive 1 as indicated below. The output is stored on drive 0 in unnormalized (40,40) binary floating-point numbers, and each sequence of answers is followed by $\sum \eta(x,t)$, which may or may not be a good approximation of $b \int \eta(x,t) dx$, depending on b . The usual (40,40) output routine converts unnormalized as well as normalized numbers. The quantity $A(x) \neq 0$ for any x , and should this not be the case, a small number should replace that particular value. "Small" here means that if $A(x) = 0$, then replace $A(x)$ by $b A(x-b)$ or $b A(x+b)$, whichever is smaller, where b is in the range of 0.1 to 0.001. Extremely small values of b could cause scaling trouble of insurmountable proportions. The input numbers are in (40,40) binary floating-point (preferably normalized for accuracy), binary fractions, and hexadecimal integers as indicated below.¹ The one exception is that 0

¹Codes are written to take care of setting up the input and securing the output.

in (40,40) binary must have an exponent of zero [contrary to the usual (40,40) input conversion routine]. The only coded stops are (1) R_k is not digital, (2) $M_0 = N_0 = 0$, (3) $M_N = N_N = 0$. The code will continue to compute $\eta(x,t)$ for consecutive time intervals until

$$\left| \frac{\sum \eta(x,t - \Delta t)}{\sum \eta(x,t)} - 1 \right| < \epsilon .$$

When this condition is satisfied the code stops in address 0A1. The output should then be secured.¹

If Δt is large (of order 10^{15} , say) and $g = 0$, Eq. (4) reduces to the ordinary differential equation

$$\eta'' + \frac{B}{A} \eta' + \frac{C}{A} \eta + \frac{2D}{A} = 0 .$$

Hence to solve

$$A\eta'' + B\eta' + C\eta + D = 0 ,$$

A , B , and C are stored as if they were coefficients of a partial differential equation but $D/2$ is stored instead of D . Also ϵ (the convergence constant) should be chosen greater than 1 since the code must stop after the first iteration. The solution sought is the second set of output data.

Code Limits and Restrictions

1. $A(x) \neq 0$ (see above discussion).
2. $x \neq 0$ (this applies to all x ; a small variation in x should suffice).
3. The maximum number of mesh points is 150 (decimal).

Time Approximations

Partial Differential Equation: After initial setup, between four and eight time intervals are calculated per minute, depending on the number of mesh points.

Ordinary Differential Equation: About 1 min is required for each such solution.

The Coded Stops

1. R_k is not digital: The mesh is too large for a good approximation of the derivatives of the coefficients to be obtained.
2. $M_0 = N_0 = 0$: This does not constitute a boundary condition.
3. $M_N = N_N = 0$: This does not constitute a boundary condition.

Magnetic Tape Drives

Drive 0: Setup numbers and output are stored here. Information is not saved from case to case.

Drive 1: Input information is stored here. Tape is not written on or rewound.

Drive 2: Intermediate results are stored here.

Drive 3: SOL is stored here (26 hex blocks). To set up additional code, another 1D (hex) blocks are used.

The input storage sequence is shown in Table 1, and the output sequence in Table 2.

Operating Instructions

The block counter of drives 0 and 2 must be 0. Drive 1 is set at the beginning of input and drive 3 is at the beginning of the code.

1. Read one block from drive 3 into 000.
2. Transfer to left of 000.
3. Operate.

Restarting Instructions

If after the first few minutes in operation an error occurs which cannot be corrected or if the solution is incomplete, the code may be restarted as follows:

1. Set block counter of drive 3 to 026, relative to beginning of code.
2. Hunt drive 0 back to a good solution with block counter reading m (say).
3. Hunt drive 2 back to m ; read in $2n + 4$ words from drive 2 to 6D0.
4. Hunt drive 2 back $4n + 8$ words, $2n + 4$ at a time.
5. Read in 6D0 words from drive 3 to 000.
6. Transfer to left of 005.

4. NUMERICAL EXAMPLES AND COMMENTS

The following differential equations were used to check SOL.

Problem 1:

$$\frac{\partial \eta}{\partial t} = x^2 \frac{\partial^2 \eta}{\partial x^2} + x \frac{\partial \eta}{\partial x} - 5\eta + x, \quad 2 \leq x \leq 3,$$

with boundary conditions

$$2 \frac{d\eta}{dx} - 2\eta = 0 \quad \text{at } x = 2,$$

$$3 \frac{d\eta}{dx} - 2\eta = 0 \quad \text{at } x = 3,$$

and solution

$$\eta = x^2 (1 - e^{-t}).$$

Table 1. Input Information (Drive 1)

	1st Bk.	2nd Bk.	3rd Bk.	...	jth Bk.	...	kth Bk.	...	mth Bk.
000	0	M_0	$A(x)$	...	$B(x)$	...	$C(x)$	...	$D(x)$
001	$x(\text{int})$	N_0	exp.		exp.		exp.		exp.
002	exp.	L_0	$A(x+b)$		$B(x+b)$		$C(x+b)$		$D(x+b)$
003	b	M_N	exp.		exp.		exp.		exp.
004	exp.	N_N	.		.		.		.
005	g	L_N	.		.		.		.
006	exp.		.		.		.		.
007	$n(\text{hex})$								
008	Δt								
009	exp.								
024	ϵ								
025	exp.								

Notes:

 $x(\text{int})$ - the initial value of the variable x . b - the increment in x . g - a constant; usually zero but has application in reactor problems. n - the number of mesh points in hexadecimal. Δt - the increment in t . ϵ - convergence constant. $M_0, N_0, L_0, M_N, N_N, L_N$ - binary fractions.

All numbers with exponents are in (40, 40) binary floating-point.

Table 2. Output (Drive 0)

1st Bk.	...	jth Bk.	...	kth Bk.	...
$\eta(x, 0) = 0$	.	$\eta(x, \Delta t)$	.	$\eta(x, t)$	.
exp.	.	exp.	.	exp.	.
$\eta(x+b, 0) = 0$	.	$\eta(x+b, \Delta t)$	.		.
exp.		.			
.	$\eta(x + [n-1]b, 0)$	.			
.	exp.	.			
.	$\sum_{i=0}^{n-1} \eta(x+ib, 0)$				
	exp.				

Problem 2:

$$\frac{\partial \eta}{\partial t} = \frac{\partial^2 \eta}{\partial x^2} + \sin n\pi x, \quad 0 \leq x \leq 1, \quad n \text{ an integer,}$$

with boundary conditions

$$\eta(0, t) = 0, \quad \eta(1, t) = 0$$

and solution

$$\eta = \frac{\sin n\pi x}{\pi^2 n^2} \left(1 - e^{-n^2 \pi^2 t} \right).$$

Problem 1 was solved using $P = Q = 1/2$, $R = 0$, $\Delta t = 1/10$, and $b = 1/10$ for 40 time intervals. At each interval the solution was in error by less than 1%. Cases were run using different values for P , Q , and R . For $P = 9/20$, $Q = 3/5$, $R = -1/20$, the solution was in error by 10% at $t = 1/5$; the error was about 1% at $t = 1$, and about 0.05% at $t = 4$. Using $P = 5/12$, $Q = 2/3$, $R = -1/12$, the solution was in error by 10% at $t = 1/5$. At $t = 1\frac{3}{5}$, the error was about 1%, but at $t = 3\frac{1}{5}$, the solution was noticeably oscillating around the true solution. The oscillation built up to errors of 25% at $t = 4$. Using $\Delta t = 10^{-15}$, the steady-state solution was in error by less than 0.1%. Problem 1 was also solved for the interval $0 \leq x \leq 2$ using $0.001 \approx 0$. No additional error occurred.

Problem 2 was solved using $P = Q = 1/2$, $R = 0$, $\Delta t = 1/100$, $(1/1000)$, $(1/10000)$, $b = 1/20$, and $n = 1, (2)$. In all cases the solution was in error by less than 1%.

To date several production problems have been run, both partial and ordinary. One problem with widely varying coefficient functions was solved using $\Delta t = 1/200$, $b = 1/200$ and also for $\Delta t = 1/10$, $b = 1/50$. The solutions varied by less than 5%. For one case R_k was not digital. This was overcome by taking half of b . One problem was run for 1000 time intervals.

APPENDIX. THE CENTRAL DIFFERENCE APPROXIMATION

A logical question arises as to why a central difference approximation was not used in approximating Eq. (28). Below it will be shown that the central difference approximation will not satisfactorily satisfy conditions A and B.

If a central difference approximation is substituted for $dT(t)/dt$ in Eq. (28), Eq. (32) becomes

$$(1 - 2\lambda P \Delta t) W^2 - 2\lambda Q \Delta t W - (1 + 2\lambda R \Delta t) = 0.$$

For any values of P , Q , and R , the absolute value of the larger root, for all λ , is not necessarily large as compared to the absolute value of the smaller. Hence, while values of P , Q , and R can be chosen on the basis of accuracy, this is no guarantee that the approximation is valid or the solutions converge, in t , to the real solution.

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