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A METHOD FOR SOLVING MOVING BOUNDARY PROBLEMS IN HEAT FLOW
PART I : USING CUBIC SPLINES.

by

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ABSTRACT

A new approach to a heat-flow problem involving a moving boundary makes use of a grid system which moves with the boundary. The necessary interpolations are performed by using cubic splines. The method smooths out irregularities in the motion of the boundary which were evident in previous calculations based on a fixed grid system.

A Method for Solving Moving Boundary Problems in Heat Flow : Part I - Using Cubic Splines.

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1. Introduction.

Previous papers have described various ways of dealing with a moving boundary in heat flow or diffusion problems. Most of them refer to a boundary on which a change of physical state occurs with the absorption or liberation of latent heat. The present authors [1] have discussed a slightly different problem presented by the diffusion of oxygen in an absorbing medium and the counterpart in heat flow is clearly of interest. An early finite-difference method [2] proposed the use of a variable time step chosen so that the boundary always moves from one line of the space grid to the neighbouring one in a single time step. Another method [3] which maintains a fixed number of equal space intervals between the moving boundary and the surface of the medium, the size of interval being correspondingly adjusted, leads to a more complicated form of the heat flow equation. It contains a parameter which is the unknown velocity of the moving boundary and is analogous to the equation which results from the use of a transformed space variable expressed as a fraction of the space coordinate of the boundary which is time-dependent. The present authors [1] used finite-difference formulae for unequal intervals in the region of the moving boundary together with a Taylor's series expansion.

In the present paper, use is made of a uniform space-grid which moves with the velocity of the moving boundary. This has the effect of transferring the unequal interval from the neighbourhood of the moving boundary to the surface of the medium. An improvement in the degree of smoothness in the calculated motion of the boundary is effected. The method discussed makes use of interpolating oubic splines.

2. An Example.

We shall introduce the new method by referring to a practical problem which the authors described in detail in the earlier paper [1]. Expressed in non-dimensional terms we require the solution of the equation

$$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2} - 1, \;\; 0 \le x \le \delta(t), \tag{1}$$

with the boundary conditions

$$\frac{\partial u}{\partial x} = 0, \quad x = 0, \qquad t \ge 0 \;, \tag{2}$$

$$u = \frac{\partial u}{\partial x} = 0, \qquad x = \delta(t), \qquad t \ge 0, \tag{3}$$

and the initial condition

$$u = \frac{1}{2}(1-x)^2, \;\; 0 \le x \le 1 \;\;, \quad t = 0 \;, \tag{4}$$

Where $\delta(t)$ denotes the position of the moving boundary at time t.

3. A Moving Grid System.

Traditionally, we divide the region $0 \le x \le 1$ into n intervals each of width Δx such that $x_i = i\,\Delta x$, i = 0,1, ... n and $n\,\Delta x = 1$. By some numerical procedure we advance the solution in finite time steps Δt, starting from the known solution at t = 0, given by(4).

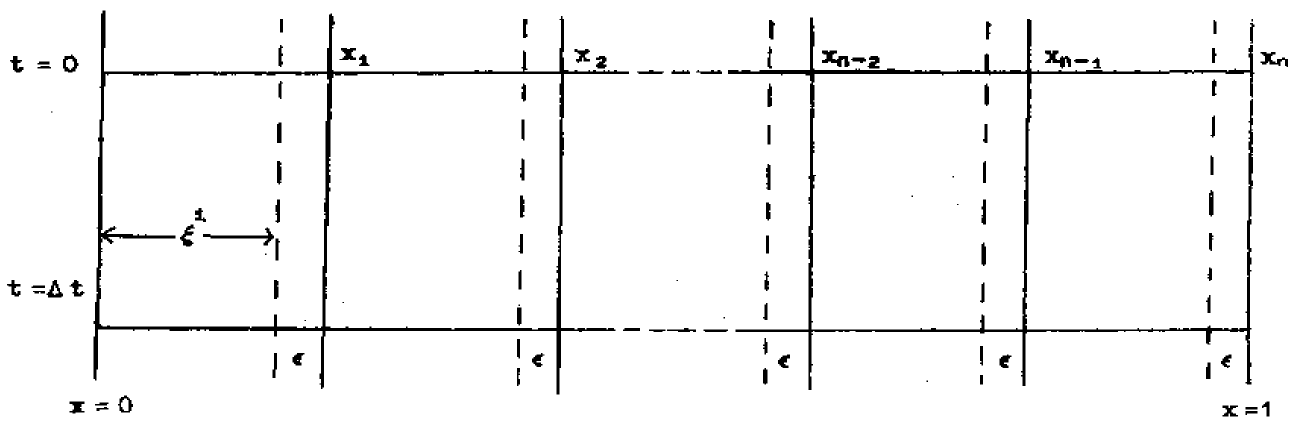

Fig. 1. Moving Grid.

We denote by U_i^j the values of u at $(i\,\Delta x, j\Delta t)$, j = 0, 1, 2 ...., so that in the first interval Δt we evaluate U_{n-1}^1 and also the new position of the boundary which has moved from x = 1 to x= 1-∈, say, as in Figure 1. We now move the whole grid a distance ∈ to the left as indicated by the broken lines, and we wish to evaluate values of U^o and the second space derivatives at each of the points x_1 -∈, x_2 -∈, ... x_{n-1} -∈, 1-∈. We describe below a method of doing this, using cubic splines for interpolating between the points x_0, x_1 , x_2 .... X_{n-1} , 1 at t = 0. We can then proceed in similar fashion to $2\,\Delta t$ and in general to $j\,\Delta t$ (j = 3,4,....) provided we include a modification to allow for the unequal interval ξ^j at the jth time step near the surface x = 0.

4 Forward-Difference Spline (F.D.S.) Method.

We base our interpolations in $x_j < x < x_{j+1}$, i = 0,2,3, ... n - 1, on the cubic spline given by

$$s(x) = U_j + (x - x_j) \left\{ \frac{U_{i+1} - U_i}{x_{i+1} - x_i} - \frac{1}{6}(x_{i+1} - x_i)\big(2S''(x_i) + x''(x_{i+1})\big) \right.$$

$$\left. + \frac{1}{2}(x - x_i)^2 S''(x_i) + \frac{1}{6}(x - x_i)^3 \left\{ \frac{S''(x_{i+1}) - s''(x_i)}{x_{i+1} - x_i} \right\} \right., \quad (5)$$

where $S''(x_j)$ denote the second derivatives at x_j, (i = 0, 1, 2, ... n -1).

These are determined from the following tridiagonal set of equations

$$(x_i - x_{i-1})\, S''(x_{i-1}) + 2(x_{i-1} - x_{i-1})\, S''(x_i) + ((x_{i+1} - x_i)\, S''(x_{i+1})$$

$$= 6\left\{ \frac{U_{i+1} - U_i}{x_{i+1} - x_i} - \frac{U_i - U_{i-1}}{x_i - x_{i-1}} \right\}, \quad (6)$$

i = 1, 2, ... n-1.

The equations express the continuity of the first derivatives $S'(x_L)$. They form a set of only n-1 equations while there are n + 1 unknown function values to be evaluated. We derive two further relationships from the given boundary conditions.

Differentiating (5) with respect to x and using (2) we find

$$2S''(x_o) + S''(x_2) = \frac{6(U_1 - U_o)}{(x_1 - x_0)^2} = \frac{6(U_1 - U_0)}{\xi^2} . \qquad (7)$$

Similarly at the moving boundary, $\delta(t)$, we can find a relation given by

$$S''(x_{n-1}) + 2\,S''(x_n) = \frac{6U_{n-1}}{\Delta x^2} . \qquad (8)$$

But we have also shown in [1] that

$$\frac{\partial^2 u}{\partial x^2} = 1 , \quad \frac{\partial^3 u}{\partial x^3} = -\frac{d\delta}{dt} , \quad \frac{\partial^4 u}{\partial x^4} = \left(\frac{\partial\delta}{dt}\right)^2 \text{ etc. at} \qquad (9)$$

The moving boundary, giving $S''(x_n) = 1$.

Since we make use of (9) later on, to determine the position of the moving boundary, we prefer to include it rather than (8) in the solution of the tridiagonal set of equations given by (6). Having determined the second derivatives at the given points or knots, the values of u(x) at intermediate points can be found from (5). The second derivatives at the intermediate points are readily available, for a cubic spline, by linear interpolation between the knots.

Assuming the function values to be known' at any time $j\Delta t$ when the distance of the moving boundary from the surface x = 0 is $\xi^j + r\Delta x$, the method proceeds as follows. Obtain the second derivatives $S''(x_i)$, i = 0,1 , ... ,(r + 1) by solving the tridiagonal set (6) together with (7) and (9) . The value of U_r^{j+1} i.e. at the point neighbouring the moving boundary, follows from the simple explicit relationship

$$\frac{U_r^{j+1} - U_r^j}{\Delta t} = S''\ (x_r^j)\ - 1\ , \tag{10}$$

where $S''(x_r^j)$ denotes the value of the second derivative at x_r at $t = j\Delta t$.

The Taylor's series for U_r obtained by expanding about the moving point can be written as

$$U_r = U\left(\delta\right)\ell\left(\frac{\partial u}{\partial x}\right)_{x=\delta} + \tfrac{1}{2}\ell^2\left(\frac{\partial^2 u}{\partial x^2}\right)_{x=\delta} - \frac{1}{6}\ell^3\left(\frac{\partial^3 u}{\partial x^3}\right)_{x=\delta} + \ ....,$$

where $\ell\,(0 \le \ell \le \Delta\ x)$ is the distance of the moving point from U_r.

Using (3) and (9) and assuming that the boundary is not moving too quickly, the above relation gives to a reasonable accuracy

$$\ell = \sqrt{(2U_r)}\ . \tag{11}$$

Therefore, once U_r^{j+1} is known from (10), we can find the position of the moving boundary from (11). Hence, the movement, $\in^{j+1}$, of the boundary in time At, from $j\Delta t$ to $(J + 1)\ \Delta t$ is given by

$$\in^{j+1} = \Delta x - \ell^{j+1}\ . \tag{12}$$

Having got $\in$ from (12) we then interpolate the values of $u(x)$ at $t = j\Delta t$ at the points $x_1 - \in$, $x_2 - \in$, ... , $x_r - \in$, $\delta - \in$

using (5) and the corresponding second derivatives from the linear relationship

$$\frac{S''(x_{i+1}^{j}) - S''(x)}{x_{i+1}^{j} - x} = \frac{S''(x_{i+1}^{j}) - S''(x_{i}^{j})}{x_{i+1}^{j} - x_{i}^{j}} , \qquad (13)$$

where x_i^j denotes the ith mesh point such that $x_i^j = \xi^j + (i-1)\Delta x$ at time $j\Delta t$; $x_i^j \le x \le x_{i+1}^j$ and i = 0, 1 , ..., r.

The values of u(x) at x_1, x_2,.....x_r, at time (j+1) Δt follow at once from

$$\frac{U^{j+1}(x_i^{j+1}) - U^{j}(x_i^{j} - \in^{j+1})}{\Delta t} = S''(x_i^{j} - \in^{j+1}) - 1 , \qquad (14)$$

$$x_i^{j+1} = x_i^{j} - \in^{j+1} , \qquad i = 1,2,.....r.$$

together with

$$\frac{U_o^{j+1} - U_o^{j}}{\Delta t} = S''(x_o^{j}) - 1 \text{ , at the surface } x = 0. \qquad (15)$$

We should remember that the space interval x_1 - x_0 = ξ is not fixed and varies from one time step to the next.

Proceeding in steps At in this way we eventually find that the points x_0 and x_1 come so close together that the values of u there are not significantly different, to the'accuracy of working. We then replace ξ by $\Delta x + \xi$ to get values at the next time step and proceed as before.

5. Results and Discussion.

In our previous paper [1], an analytical solution satisfactory for small times was obtained which is given by

$$u(x,t) \simeq \frac{1}{2}(1-x)^2 - 2\sqrt{\left(\frac{t}{\pi}\right)} \exp\left\{-\left(\frac{x}{2\sqrt{t}}\right)^2\right\} + x\,\mathrm{erfc}\left(\frac{x}{2\sqrt{t}}\right), \tag{16}$$

$$0 \le x \le 1 \text{ and } t \text{ small}$$

We start the present solution from the values taken from (16) at t = 0.025 when the boundary $\delta = 1$, has not moved to an accuracy of six significant figures [1]. The positions of the moving boundary and the surface concentrations have been computed by the FDS method and are compared 3n Tables I and II respectively, with the corresponding values obtained from the previous method of [1] which from now on we call the Fixed Grid Lagrange (FG-L) method. The values show a reasonably good agreement between the two methods. We are not able to assess the accuracy of the results by a rigorous analysis so we have quoted results by the FGL method for $\Delta x = 0.05$ as well as for $\Delta x = 0.10$. The surface values of u are in good agreement. The calculated positions of the moving boundary agree reasonably well until the concentrations are everywhere quite small.

Now let us consider the major problem of roughness in the positions of the moving boundary which is produced by the FGL method near the times when the process used to calculate the concentration in the neighbourhood of the moving point is transferred one space interval towards the surface x = 0. Table III gives the positions of the boundary at and around such times of shifting the interval in the FGL method, along

TABLE I

Comparison of $10^4\delta$ at different times. The numerical solutions start from the analytical solution at t = 0.025.

Method \ Time	0.040	0.060	0.100	0.120	0.140	0.160	0.180	0.185
FGL $\Delta x = 0.10$	9988	9905	9312	8747	7912	6756	4849	4014
FGL $\Delta x = 0.05$	9992	9918	9346	8781	7966	6799	4942	4178
FDS $\Delta x = 0.10$	9993	9920	9327	8739	7892	6664	4680	3917

TABLE II

Comparison of 10^4 U at the surface x = 0, at different times. The numerical solutions start from the analytical solution at t = 0.025.

Method \ Time	0.040	0.060	0.100	0.120	0.140	0.160	0.180	0.185
FGL $\Delta x = 0.10$	2745	2238	1434	1094	781	490	220	156
FGL $\Delta x = 0.05$	2742	2234	1430	1089	777	486	216	151
FDS $\Delta x = 0.10$	2736	2277	1424	1083	771	481	210	145

TABLE III

Table showing the irregularities in the position of the moving boundary, calculated by the FGL method. Comparatively smooth figures are shown for the FDS method ($\Delta x = 0.10$)

Time	FGL Method			FDS Method		
	$10^4\delta$	$-\Delta$	$-\Delta^2$	$10^4\delta$	$-\Delta$	$-\Delta^2$
0.110	9099 9070 9040 9010 8984	29 30 30 26	1 0 4	9118 9090 9061 9031 9001	28 29 30 30	1 1 0
0.137	8141 8089 8034 7994 7954	52 55 40 40	3 -15 0	8133 8086 8039 7991 7942	47 47 48 49	0 1 1
0.154	7277 7204 7124 7037 6985	73 80 87 52	7 7 -35	7214 7150 7085 7018 6950	64 65 67 68	1 2 1
0.167	6396 6306 6203 6045 5979	90 103 158 66	13 55 -92	6266 6180 6093 6003 5910	86 87 90 93	1 3 3
0.176	5499 5393 5268 5020 4937	106 125 248 83	19 123 -165	5406 5296 5181 5063 4940	110 115 118 23	5 3 5
0.184	4652 4538 4406 4014 3912	114 132 392 102	18 260 - 290	4397 4245 4085 3917 3738	152 160 168 179	8 8 11

NOTE: The data are tabulated at an interval of time $\Delta t = 0.001$. The underlined values correspond to the times when the interpolation process near the moving boundary is transferred one step to the left.

TABLE IV

Table showing the smoothness of the surface concentrations calculated by the FDS method. Comparative figures are given for the FGL method ($\Delta x = 0.10$).

Time	FGL Method		FDS Method	
	$10^4 U_o$	$-\Delta$	$10^4 U_o$	$-\Delta$
0.105	1371		1381	
		18		18
	1353		1363	
		17		17
	<u>1336</u>		1346	
		18		18
	1318		1328	
		17		17
	1301		1311	
0.136	862		872	
		15		16
	847		856	
		15		15
	<u>832</u>		841	
		16		15
	816		826	
		15		15
	801		811	
0.154	594		604	
		14		14
	580		590	
		14		15
	<u>566</u>		575	
		15		14
	551		561	
		14		14
	537		547	
0.167	411		421	
		13		14
	398		407	
		14		14
	<u>384</u>		<u>393</u>	
		14		13
	370		380	
		13		14
	357		366	
0.177	276		286	
		13		14
	263		272	
		13		13
	<u>250</u>		<u>259</u>	
		14		13
	236		246	
		13		13
	223		233	
0.184	184		194	
		13		13
	171		181	
		13		13
	<u>158</u>		168	
		13		13
	145		155	
		12		12
	133		143	

NOTE: The data are tabulated at an interval of time $\Delta t = 0.001$. The underlined values correspond to the times given in the first column, when the first space interval is increased by Δx.

with the corresponding figures from the FDS method. The irregularities produced in the former method are clearly visible, whereas their counterparts show a smooth behaviour throughout.

Table IV gives the surface concentrations computed from the present method at and around the times when the first space interval ξ is increased to $\xi + \Delta x$ for the succeeding computations. It is interesting to note that the differences in the concentrations show no sign of irregularities. The comparative figures from the PGL method are also given in Table IV.

It has also been noted that the results obtained by using (8) instead of (9) are very close.

6 Generalisation

Let us consider a problem in heat flow in which a change of 3tate occurs with latent heat on a moving boundary. In non-dimensional form the relevant equations are

$$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2} , \quad 0 \leq x \leq \delta (t) \quad ; \tag{17}$$

$$\frac{\partial u}{\partial x} = -1 , \quad x = 0, \; t > 0 \quad ; \tag{18}$$

$$u = 0 , \quad x = \delta(t), \; t \geq 0 \quad ; \tag{19}$$

$$\frac{\partial u}{\partial x} = - \frac{\partial \delta}{\partial t} = - \dot{\delta} \quad x = \delta (t) \quad ; \tag{20}$$

$$\delta = 0, \quad t = 0. \tag{21}$$

In order to get a solution of the tridiagonal set of equations (6) we need to know two more equations involving second derivatives at the grid points. We replace the surface condition (18) by an equation corresponding to (7) which is given by

$$2\,S''(X_O) - S''(X_1) = \frac{6}{\xi^2}(U_1 - U_0) + \frac{6}{\xi} . \tag{22}$$

By differentiating (19) with respect to t and using (17) and (20) it is easy to show that

$$\left(\frac{\partial^2 c}{\partial x^2}\right)_{x=\delta} = \left(\frac{\partial \delta}{\partial t}\right)^2 = \dot{\delta}^2 , \tag{23}$$

giving $S''(x_n) = \dot{\delta}^2$ where $\dot{\delta}$ is a function of time t. Let us assume that the values of U_0, U_1 .... U_r, U_{r+1} are known at the jth time level and the position of the moving boundary is also known at that time which is given by $\delta^j = \xi^j + r\Delta x$. The width of all the meshes is Δx except the first one which is ξ^j.

The Taylor's expansion for U_r about the moving boundary can be written as

$$U_r = (U)_{x=\delta} - \Delta x \left(\frac{\partial u}{\partial x}\right)_{x=\delta} + \frac{1}{2}\Delta x^2 \left(\frac{\partial^2 u}{\partial x^2}\right)_{x=\delta} \cdots\cdots ,$$

which after substituting from (20) and (22) gives

$$\dot{\delta} = -1 + \sqrt{1+2U_r} . \tag{24}$$

By putting value of $\dot{\delta}$ from (24) in (23), we get

$$S''\ (x_{r+1}) \quad = \quad (-1 + \sqrt{1+2U_r})^2 \quad . \qquad (25)$$

The tridiagonal set of equation (6) together with (22) and (25) can now be solved giving the second derivatives at $x_0, x_1, \ldots. x_r, \ldots. x_r, x_{r+1}$ at time (j + 1) Δt at time j Δt.

The relation (24) also gives the new value of δ i.e. δ^{J+1} at time (j + 1) Δt after replacing $\dot{\delta}$ by a forward finite difference i.e.

$$\frac{\delta^{j+1} - \delta^j}{\Delta t} = -1 + \sqrt{1+2U_r^j} \quad . \qquad (26)$$

The desired interpolation for the value of U and its second derivatives can then be oarried out as described in section 4. It should, however, be mentioned here that the boundary δ(t) is moving forward i.e. away from the surface x = 0. In this situation the first interval ξ is to be "broken into two when it becomes larger than Δx. The new interval near the surface will then be of width ξ - Δx. The value of u, at the new mesh point, has to be interpolated using (5).

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