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Technical Note

Numerical treatment of rapidly changing and discontinuous conductivities

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Abstract

The Kirchhoff transformation is an effective means for dealing with temperature dependent conductivities. In general numerical applications, however, the use of this approach will produce non-linear discrete equations, which can be costly to solve. This paper introduces a local Kirchhoff approach for approximating the conductivity terms in the discrete equation. This approach results in an efficient solution in terms of temperature alone. Application to a problem with rapidly changing conductivity shows that use of high-order numerical integration in the conductivity approximation leads to very accurate predictions. © 2001 Elsevier Science Ltd. All rights reserved.

1. Introduction

In the numerical solution of diffusion-controlled heat and mass transfer problems an area that often leads to difficulty is the treatment of conductivities that are strong functions of the dependent variable. In the context of phase change problems, with a sharp front and a discontinuous change in conductivity, e.g., the melting or solidification of a pure material, a number of numerical schemes have been proposed [1,2]. Voller and Swaminathan [2] develop a scheme based on a local Kirchhoff transformation [3]. The objective of this short note is to extend the local Kirchhoff approach introduced by Voller and Swaminathan [2] to a case where the conductivity is a continuous but strong function of the dependent variable. Such behavior can be associated with phase change problems that exhibit so-called "mushy" regions, e.g., the solid–liquid dendritic region in a binary alloy [4] or unsaturated moisture migration through soil [5].

2. The local Kirchhoff method

Heat conduction is chosen as an example diffusion process to illustrate the method development. The governing equation for a transient heat conduction process in a given volume is

$$\rho c \frac{\partial T}{\partial t} = \nabla \cdot [K(T) \nabla T] + S, \tag{1}$$

where suitable boundary conditions are applied at the surface of the volume, ρ is the density, c is the specific heat, $K(T)$ is a temperature-dependent conductivity, and S is a source term. Any problems that may occur due to a rapidly changing or discontinues $K(T)$ can be bypassed by using a Kirchhoff transformation [3]

$$\phi = \int_0^T K(\xi)\, \mathrm{d}\xi. \tag{2}$$

By the Leibniz rule,

$$\nabla \cdot [K \nabla T] = \nabla^2 \phi, \tag{3}$$

so that Eq. (1) can be written as

$$\rho c \frac{\partial T}{\partial t} = \nabla^2 \phi + S. \tag{4}$$

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Any volume-based discretization of Eq. (4) can be written in the general point form

$$\sum_i a_i(\phi_P - \phi_i) + S_P T_P = S_C, \tag{5}$$

where the summation is over the nodes that "neighbor" node P (see the section of the 2-D finite element grid in Fig. 1), the a_i are constant coefficients, with values determined by the nature of the discretization and the order of approximating interpolation used. The transients, source terms and boundary conditions are represented by the source coefficients S_P and S_C in Eq. (5). The obvious problem in using Eq. (5) is that it is nonlinear and, depending on the form of $K(T)$, considerable work may be required to solve it. In cases where the form of $K(T)$ leads to an "awkward" definition of the Kirchhoff variable the alternative direct discretization of Eq. (1), i.e.,

$$\sum_i a_i K_{P-i}(T_P - T_i) + S_P T_P = S_C, \tag{6}$$

may be a more attractive option. In Eq. (6) the term K_{P-i} is an appropriate average value of $K(T)$ controlling the heat transfer between node P and its neighbor node i. A direct equivalence between Eqs. (5) and (6) can be made on noting that if s is the unit vector in the direction of the line joining node P to node i

$$K_{P-i} = \frac{\mathrm{d}\phi}{\mathrm{d}s} \bigg/ \frac{\mathrm{d}T}{\mathrm{d}s}. \tag{7}$$

With this definition of K_{P-i} a solution of Eq. (6) will be equivalent to solving the Kirchhoff form in Eq. (5). The advantage of this local application of the Kirchhoff transformation is that, if an appropriate discrete form of Eq. (7) is used, there will be no ambiguity in the treatment of $K(T)$. A central difference approximation of Eq. (7) is

$$K_{P-i} = \frac{\phi_P - \phi_i}{T_P - T_i}. \tag{8}$$

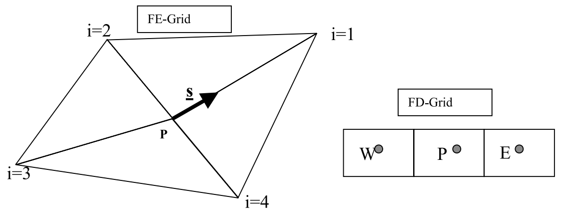

Fig. 1. Examples of a finite element and finite difference grid.

In a case where $K(T)$ is discontinuous at a fixed temperature (scaled to be $T = 0$) with constant values ($K = K_{\mathrm{sol}}$ if $T < 0$ and $K = K_{\mathrm{liq}}$ if $T > 0$) on both sides of the discontinuity Eq. (8) becomes

$$K_{P-i} = \frac{KT_P - KT_i}{T_P - T_i}, \tag{9}$$

which is the "state of face" conductivity proposed and tested by Voller and Swaminathan [2] for solid–liquid phase change problems that exhibit a discontinuity in the conductivity at the phase change temperature. In a case where $K(T)$ is continuous but undergoes rapid changes Eq. (8), with reference to the definition of the Kirchhoff transformation in Eq. (2), can be written as

$$K_{P-i} = \frac{\int_{T_i}^{T_P} K(\xi)\,\mathrm{d}\xi}{T_P - T_i}. \tag{10}$$

Clearly a direct evaluation of the integral in the numerator of Eq. (10) can be made. An alternative is to use numerical integration and approximate the numerator as

$$\int_{T_i}^{T_P} K(\xi)\,\mathrm{d}\xi \approx \left[T_p - T_i\right] \sum w_j K(g_j), \tag{11}$$

where w_j are the weights and g_j are the integration points in the interval $\{T_p, T_i\}$. In this way

$$K_{P-i} = \sum w_j K(g_j). \tag{12}$$

The use of Eq. (12) in Eq. (6) is the main result in this paper. Its use allows for a direct temperature-based solution of the governing diffusion equation which treats variations in $K(T)$ at the level of accuracy offered by the Kirchhoff transformation. Specific forms of Eq. (12), based on the various integration rules, are listed in Table 1; the accuracy of the approximation controlled by the order of the integration rule used.

Table 1
List of integration rules for use in Eq. (12)

Integration scheme	Integration points	Integration weights
Mid-point	$g_1 = \frac{T_P+T_i}{2}$	$w_1 = 1$
Trapezoidal	$g_1 = -T_P, \quad g_2 = T_i$	$w_1 = \frac{1}{2}, \quad w_2 = \frac{1}{2}$
Two-point Gauss	$g_1 = \frac{-1}{\sqrt{3}}\frac{T_P-T_i}{2} + \frac{T_P+T_i}{2}, \quad g_2 = \frac{1}{\sqrt{3}}\frac{T_P-T_i}{2} + \frac{T_P+T_i}{2}$	$w_1 = \frac{1}{2}, \quad w_2 = \frac{1}{2}$
Three-point Gauss	$g_1 = \frac{-\sqrt{3}}{\sqrt{5}}\frac{T_P-T_i}{2} + \frac{T_P+T_i}{2}, \quad g_2 = \frac{T_P+T_i}{2}, \quad g_3 = \frac{\sqrt{3}}{\sqrt{5}}\frac{T_P-T_i}{2} + \frac{T_P+T_i}{2}$	$w_1 = \frac{5}{18}, \quad w_2 = \frac{8}{18}, \quad w_3 = \frac{5}{18}$

3. A test problem

The key features of the proposed approach can be sufficiently demonstrated by considering the following steady one-dimensional heat diffusion problem

$$\frac{\mathrm{d}}{\mathrm{d}x}\left[K(T)\frac{\mathrm{d}T}{\mathrm{d}x}\right] = 0, \quad 0 \leqslant x \leqslant 1 \tag{13}$$

with $T(0) = 0$, $T(1) = 2$ and the conductivity specified by

$$K = \frac{1}{1 + T^6} \tag{14}$$

a function which is plotted in Fig. 2. An analytical solution for this problem can be readily obtained in terms of the Kirchhoff transformation

$$\phi = 1.041x \tag{15}$$

from which $T(x)$ can be determined by inverting

$$\begin{aligned}\phi &= \int_0^T K(\xi)\,\mathrm{d}\xi \\ &= \frac{\tan^{-1}(T)}{3} - \frac{\sqrt{3}}{12}\ln\left(T^2 - \sqrt{3}T + 1\right) \\ &\quad + \frac{\tan^{-1}(2T - \sqrt{3})}{6} + \frac{\sqrt{3}}{12}\ln\left(T^2 + \sqrt{3}T + 1\right) \\ &\quad + \frac{\tan^{-1}(2T + \sqrt{3})}{6}.\end{aligned} \tag{16}$$

A numerical solution of Eq. (13) has the point form (see Fig. 1)

$$K_{P-W}(T_P - T_W) + K_{P-E}(T_P - T_E) = 0. \tag{17}$$

A standard treatment of the conductivities in Eq. (17) could use a central difference approximation

$$K_{P-W} = \frac{K(T_W) + K(T_P)}{2}, \tag{18}$$

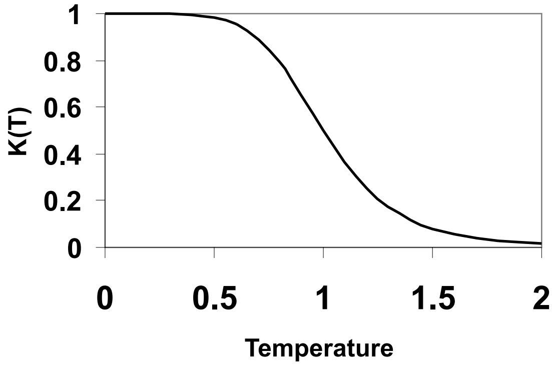

Fig. 2. Plot of conductivity against temperature.

which is the scheme that will result when a trapezoidal rule is used in Eq. (12) (see Table 1). According to the work presented here a more accurate approximation will result if a higher-order integration rule is used in Eq. (12), e.g., a two-point Gauss,

$$\begin{aligned}K_{P-W} = \frac{1}{2}\Bigg[&K\left(\frac{T_P - T_W}{2}\frac{1}{\sqrt{3}} + \frac{T_P + T_W}{2}\right) \\ &+ K\left(\frac{T_W - T_P}{2}\frac{1}{\sqrt{3}} + \frac{T_P + T_W}{2}\right)\Bigg].\end{aligned} \tag{19}$$

With reference to Fig. 3, in using a 11-node numerical solution, there is a clear improvement, in terms of comparing with the analytical solution, when Eq. (19) is used in place of Eq. (18) to approximate the conductivity. This is confirmed by plotting the relative errors

$$\%\text{Error} = 100\left|1 - \frac{T(x)}{T_P}\right| \tag{20}$$

for each of the integration schemes listed in Table 1, see Fig. 4. Basic approximate schemes for the K_{P-i} terms based on a central or mid-point averages are clearly inferior with errors well above 1% and approaching a maximum above 10%. On the other hand, the use of

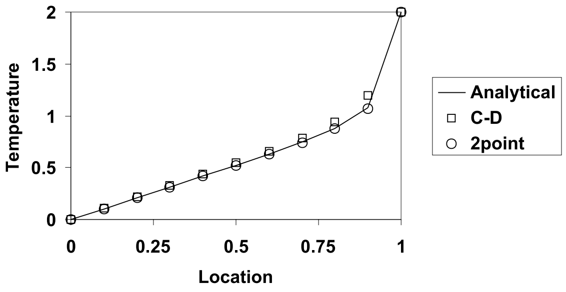

Fig. 3. Comparison of central difference and two-point Gauss approximations with analytical solution.

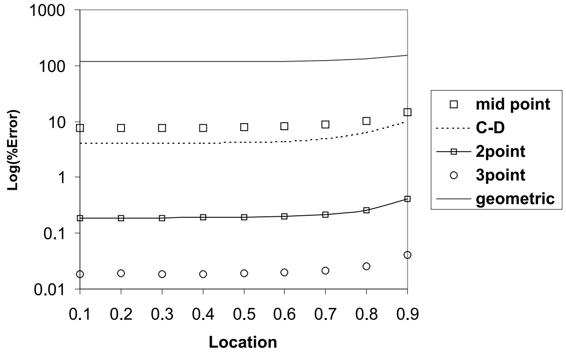

Fig. 4. Log of relative errors using each of the approximation schemes in Table 1.

more accurate integration schemes (e.g., two-point or three-point Gauss) will reduce the error well below 1%.

When the conductivity is a rapidly changing function of space, depending on the location of node points, one could argue that a geometric mean

$$K_{P-W} = \left[\frac{0.5}{K(T_W)} + \frac{0.5}{K(T_P)}\right]^{-1} \tag{21}$$

would be a good approximation for the average conductivity. As noted by Voller and Swaminathan [2], however, this form of approximation is not suitable when K is a function of the dependent variable. To confirm this the relative errors arising from a 11-node solution using the geometric approximation in Eq. (21) is also plotted in Fig. 4. It is noted that very large errors $\sim$100% occur when this approximation is used.

4. Discussion

In a numerical solution the obvious way of dealing with a variable conductivity is to employ a central difference approximation for $K(T)$. In cases where $K(T)$ changes rapidly or is discontinuous such an approximation may suffer from loss of accuracy. An alternative approach in this situation is to use a Kirchhoff transformation. This will lead to a high accuracy in the treatment of $K(T)$ but its implementation could be awkward and require a costly inversion of the transformation for the treatment of sources, transients, and boundary conditions. This paper shows how a local application of a Kirchhoff transformation can retain the directness of the first method and, if high-order numerical integration is used, approach the accuracy of the second.

In using the local Kirchhoff approximation (Eq. (12)) in Eq. (6) three key points to note are:

1. When a trapezoidal integration rule is used the method will default to a central difference scheme for $K(T)$.
2. The approach is applied after the calculation of the diffusion coefficients. In a code where the user can gain ready access to these coefficients – initially obtained by simply assuming a constant $K = 1$ in the coefficient calculation sub-routine – this approach may be quite convenient. In an iterative solution this will only require a recalculation, at each iteration, of the conductivities K_{P-i} and not the diffusion coefficients, a_i.
3. In a case where a central difference approximation is of sufficient accuracy, an application of the local Kirchhoff scheme will result in a final discretization scheme different from, and based on the analysis presented here, more accurate than a conventional scheme that uses a central difference approximation for K at the element integration points (e.g., the mid-face points in a control volume finite element scheme) directly in the calculation of the diffusion coefficients.

References

[1] S.L. Lee, R.Y. Tzong, An enthalpy formulation for phase change problems with a large thermal diffusivity jump across the interface, Int. J. Heat Mass Transfer 34 (1991) 1491–1502.

[2] V.R. Voller, C.R. Swaminathan, Treatment of discontinuous thermal conductivity in control-volume solutions of phase-change problems, Numer. Heat Transfer 24B (1993) 161–180.

[3] J. Crank, Free and Moving Boundary Problems, Clarendon Press, Oxford, 1984.

[4] C.R. Swaminathan, V.R. Voller, Towards a general numerical scheme for solidification systems, Int. J. Heat Mass Transfer 40 (1997) 2859–2868.

[5] M.A. Celia, E.T. Bouloutas, R.L. Zarba, A general mass-conservative numerical solution for the unsaturated flow equation, Water Resour. Res. 26 (1990) 1483–1496.