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Technical Notes

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Monte Carlo Solution of Transient Heat Conduction in Anisotropic Media

Farshad Kowsary* and Saeed Irano†
University of Tehran, 19858 Tehran, Iran

Nomenclature

c = specific heat capacity, J/kg · °C
dy = differential in y direction, m
F = parameter as defined by Eq. (22)
h = heat-transfer coefficient, W/m^2 · °C
$\hat{h}$ = parameter as defined by Eq. (21), m^{-1}
I = probability interval
i = number of rows
i_0 = row number from which the random walk is initiated
j = number of columns
j_0 = column number from which the random walk is initiated
k_0 = reference conductivity, W/m · °C
k_{11} = thermal conductivity in the x direction, W/m · °C
k_{12} = thermal conductivity in the xy direction, W/m · °C
$\hat{k}_{12}$ = anisotropic thermal conductivity as given by Eq. (4)
k_{22} = thermal conductivity in the y direction, W/m · °C
L = length, m
m_n = number of steps in each random walk
m_0 = parameter as defined by Eq. (14)
N = number of random walks
P = probability function
q_x = x component of the heat flux, W/m^2
q_y = y component of the heat flux, W/m^2
R_w = random number between 0 and 1
T = temperature, °C
T_n = temperature of neighboring nodes, °C
T_w = registered temperature at the end of random walk, °C
T_0 = initial temperature, °C
T_∞ = ambient temperature, °C
t = time, s
x = horizontal direction in Cartesian coordinate system, m
$\hat{x}$ = modified x coordinate, m
y = vertical direction in Cartesian coordinate system, m
$\hat{y}$ = modified y coordinate, m
α = thermal diffusivity, m^2/s
Δt = time step, s
ρ = density, kg/m^3

Subscripts

E = denotes east
N = denotes north
NE = denotes northeast
n = denotes neighboring node
S = denotes south
W = denotes west

I. Introduction

THE Monte Carlo method is a statistically based approach by which continuous physical phenomena are simulated using random events and laws of probability. Although the Monte Carlo method has been widely used in the field radiation heat transfer, its use in the field of conduction heat transfer has not been as widespread. A complete review of the application of the Monte Carlo method in conduction heat transfer for an isotropic medium is given by Haji-sheikh.[1] Recently, Deng and Liu[2] have utilized this method in bio-heat transfer.

The advantages of this method are that it requires minimal computer programming effort, demands relatively small computer memory, and it is particularly well suited for parallel computations as different processors need not communicate in the course of a randomly directed event. By using the Monte Carlo method in conduction heat transfer, the solution at every point can be obtained independently from the solution of the other points and the solution of the desired point at previous times, that is, one does not have to obtain a whole-domain solution to find the solution at certain desired points. This property is well suited for inverse heat-conduction computations.[3]

As mentioned, application of the Monte Carlo method to isotropic materials with different boundary conditions is discussed extensively in Ref. 1 However, recently, use of materials having directional conductivities, such as composites, has become more widespread in industry, and the need for efficient solution methods for obtaining the temperature field for these types of materials has become more evident. Exact analytical solutions are limited to very simple geometries and boundary conditions as presented in Ref. 4. For more complicated geometries, one has no choice but to resort to the commonly known numerical methods. For example, Aziz[5] and Flik and Tien[6] have used the finite difference and finite element methods, respectively, for the solution of heat conduction in anisotropic materials. Solution by the Monte Carlo method of steady-state anisotropic heat conduction was presented by Kowsary and Arabi.[7] In their paper they showed that there exists a valid range for the k_{12} conductivity term, outside of which the solution by the Monte Carlo method fails to exist as the probability coefficients become negative. This Note extends the Monte Carlo solution of the anisotropic heat-conduction equation to two-dimensional transient cases and shows that by a proper choice of the reference conductivity k_0 limitation on the size of the time step can be removed. A test case with Robin and adiabatic boundary conditions is taken into consideration, and the results obtained by the Monte Carlo method are compared with those obtained by the finite difference method.

II. Formulation

In the absence of internal heat generation, the heat-conduction equation for an anisotropic material in two dimensions is given by

$$k_{11}\frac{\partial^2 T}{\partial x^2} + k_{22}\frac{\partial^2 T}{\partial y^2} + 2k_{12}\frac{\partial^2 T}{\partial x \partial y} = \rho c \frac{\partial T}{\partial t} \tag{1}$$

Using the coordinate transformations given by

$$\hat{x} = x(k_0/k_{11})^{\frac{1}{2}}, \qquad \hat{y} = y(k_0/k_{22})^{\frac{1}{2}} \tag{2}$$

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*Associate Professor, Mechanical Engineering Department, Faculty of Engineering; fkowsari@ut.ac.ir.

†Graduate Student, Mechanical Engineering Department, Faculty of Engineering; sio279@yahoo.com.

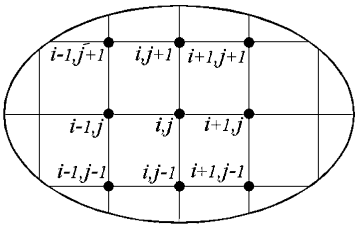

Fig. 1 Part of a mesh used in a two-dimensional geometry.

Table 1 Possible finite difference approximations of $\partial^2 T/\partial x \partial y$

No.	Equation
1	$\left(\dfrac{T_{i+1,j+1} - T_{i+1,j}}{\Delta x \Delta y}\right) - \left(\dfrac{T_{i,j+1} - T_{i,j}}{\Delta x \Delta y}\right) + \mathcal{O}\|\Delta x, \Delta y\|$
2	$\left(\dfrac{T_{i,j} - T_{i,j-1}}{\Delta x \Delta y}\right) - \left(\dfrac{T_{i-1,j} - T_{i-1,j-1}}{\Delta x \Delta y}\right) + \mathcal{O}\|\Delta x, \Delta y\|$

Eq. (1) reduces to

$$\frac{\partial^2 T}{\partial \hat{x}^2} + \frac{\partial^2 T}{\partial \hat{y}^2} + 2\hat{k}_{12}\frac{\partial^2 T}{\partial \hat{x}\partial \hat{y}} = \frac{1}{\alpha}\frac{\partial T}{\partial t} \tag{3}$$

in which $\hat{k}_{12}$ and the thermal diffusivity α are defined as

$$\hat{k}_{12} = k_{12}\Big/\sqrt{k_{11}k_{22}} \tag{4}$$

$$\alpha = k_0/\rho c \tag{5}$$

and k_0 is the conductivity at a reference temperature. As is stated by Ozisik,[4] irreversible thermodynamics dictates that the matrix of the conductivity coefficients be positive definite, which, by the definition given in this Note, translates into $k_{12} < 1$.

The derivation of the probability coefficients used in the random walk procedure in transient anisotropic problems follows the general lines of the steady-state case with some differences as shown next. Figure 1 shows an arbitrarily shaped two-dimensional body that is meshed using a rectangular grid, with $\Delta\hat{x}$ and $\Delta\hat{y}$ being the grid dimensions, respectively, in the x and y directions.

In short, the fixed-step random-walk method involves initiating a trip from a given point and following a random path according to laws of probability using the probability coefficients (derived next) and culminating the trip once an "absorbing" boundary is reached. If the temperature at the end of each trip is given by T_w and a sufficiently large number of trips are initiated from the specified point, then the temperature of that point is calculated simply by arithmetically averaging the registered temperatures at the end of each random walk. That is,

$$T(t, x, y) = \frac{1}{N}\sum_{n=1}^{N} T_W(n) \tag{6}$$

where N is the number of trips initiated from the point under consideration.

The question to be answered at this point is the manner by which a random path is determined. Once the random walker reaches a junction, the following step it will take is determined from the laws of probability using the probability functions P_n obtained as follows. The discretized form of the heat-conduction equation is written explicitly in terms of the temperature at the i, j node (i.e., the node at which the random walker is currently stationed) as

$$T_{i,j} = \sum P_n T_n \tag{7}$$

It is a clear requirement that all of these probability coefficients be nonnegative (as a negative probability is meaningless) and that they must add up to unity. As mentioned earlier, the form given by Eq. (7) is obtained by finite differencing the heat-conduction equation (1). The finite difference forms of the first two derivative terms in Eq. (3) are given by

$$\left.\frac{\partial^2 T}{\partial \hat{x}^2}\right|_{i,j} = \frac{T_{i+1,j} - 2T_{i,j} + T_{i-1,j}}{\Delta\hat{x}^2} + \mathcal{O}(\Delta\hat{x}^2) \tag{8a}$$

$$\left.\frac{\partial^2 T}{\partial \hat{y}^2}\right|_{i,j} = \frac{T_{i,j+1} - 2T_{i,j} + T_{i,j-1}}{\Delta\hat{y}^2} + \mathcal{O}(\Delta\hat{y}^2) \tag{8b}$$

To discretize the cross-derivative term $\partial^2 T/\partial\hat{x}\partial\hat{y}$, at least one of the temperatures of the nodes that are situated diagonally with respect to position of the node i, j [for example, $(i+1, j+1)$ or $(i+1, j-1)$ in Fig. 1] is needed. All possible finite difference forms of the cross-derivative term $\partial^2 T/\partial\hat{x}\partial\hat{y}$ are listed in tabular form in Ref. 9. However, from that list only those which yield nonnegative coefficients, presented in Table 1, are acceptable in Monte Carlo formulation. Arbitrarily choosing the form given in the first entry of Table 1 for the cross-derivative term, using Eqs. (8a) and (8b) for the other derivatives, substituting into the governing differential equation Eq. (3), and performing some algebraic manipulations, we would have

$$T_{i,j}^{n+1} = P_0 T_{i,j}^n + P_N T_{i,j+1}^n + P_S T_{i,j-1}^n + P_E T_{i+1,j}^n + P_W T_{i-1,j}^n + P_{\mathrm{NE}} T_{i+1,j+1}^n \tag{9}$$

$$P_W = \frac{\alpha\Delta t}{\Delta\hat{x}^2} \tag{9a}$$

$$P_S = \frac{\alpha\Delta t}{\Delta\hat{y}^2} \tag{9b}$$

$$P_N = \alpha\Delta t\left(\frac{1}{\Delta\hat{y}^2} - \frac{2\hat{k}_{12}}{\Delta\hat{x}\Delta\hat{y}}\right) \tag{9c}$$

$$P_E = \alpha\Delta t\left(\frac{1}{\Delta\hat{x}^2} - \frac{2\hat{k}_{12}}{\Delta\hat{x}\Delta\hat{y}}\right) \tag{9d}$$

$$P_{\mathrm{NE}} = \frac{2\hat{k}_{12}\alpha\Delta t}{\Delta\hat{x}\Delta\hat{y}} \tag{9e}$$

$$P_0 = \alpha\Delta t\left(\frac{1}{\alpha\Delta t} + \frac{2\hat{k}_{12}}{\Delta\hat{x}\Delta\hat{y}} - \frac{2}{\Delta\hat{x}^2} - \frac{2}{\Delta\hat{y}^2}\right) \tag{9f}$$

By inspection of Eqs. (9a–9f), it is understood that the requirement of the probability coefficients adding up to one is satisfied. It remains to look for conditions under which the probability coefficients are nonnegative. Once again examination reveals that coefficients given by Eqs. (9a), (9b), and (9e) are always nonnegative; however, appropriate criterion for the rest of the coefficients must be developed for them being nonnegative.

Equation (9d) requires that

$$\Delta\hat{y}/\Delta\hat{x} \geq 2\hat{k}_{12} \tag{10}$$

for P_E to become nonnegative. Similarly, Eq. (9c) requires that

$$\Delta\hat{y}/\Delta\hat{x} \leq 1/2\hat{k}_{12} \tag{11}$$

for P_N to be nonnegative. Combining these two equations, a permissible range for the ratio of $\Delta\hat{y}/\Delta\hat{x}$ is determined as follows:

$$2\hat{k}_{12} \leq \Delta\hat{y}/\Delta\hat{x} \leq 1/2\hat{k}_{12} \tag{12}$$

This relation also imposes a restriction on the anisotropic conductivity term. Multiplying through the inequality by $2\hat{k}_{12}$ yields $\hat{k}_{12} < \frac{1}{2}$, for which when not satisfied negative coefficients would result, and the fixed-step random walk procedure would fail to work.

Finally, for P_o to be nonnegative, Eq. (9f) requires that

$$\Delta t \leq 1\Big/\left[\alpha\left(2/\Delta\hat{x}^2 + 2/\Delta\hat{y}^2 - 2\hat{k}_{12}/\Delta\hat{x}\Delta\hat{y}\right)\right] \tag{13}$$

It was shown by Kowsary and Arabi[7] that, from the requirement that the conductivity coefficient matrices be positive definite, the expression in the parentheses must be positive. Although it appears that Eq. (13) poses a restriction on the size of the time step Δt, one notes that by a proper selection of the reference conductivity k_0, used in the definition of α in Eq. (5), this restriction can be removed.

III. Solution Algorithm

To obtain the temperature of a specified point (i_0, j_0) at a given time t, a series of random walks is initiated from that point (see Fig. 1). Imagine the random walker being positioned at the node (i, j) after a few steps. The following step of the walk depends on the probability intervals defined as

$$I_0 = [0, P_0]$$

$$I_N = [P_0, P_0 + P_N]$$

$$I_W = [P_0 + P_N, P_0 + P_N + P_W]$$

$$I_S = [P_0 + P_N + P_W, P_0 + P_N + P_W + P_S]$$

$$I_E = [P_0 + P_N + P_W + P_S, P_0 + P_N + P_W + P_S + P_E]$$

$$I_{\mathrm{NE}} = [P_0 + P_N + P_W + P_S + P_E, 1]$$

At this point a random number $R_w (0 < R_w < 1)$ is drawn, and, depending on its value, the following motions can be made:

$$R_W \in I_0 : \text{No movement}$$

$$R_W \in I_N : \text{Motion to } (i, j+1)$$

$$R_W \in I_W : \text{Motion to } (i-1, j)$$

$$R_W \in I_S : \text{Motion to } (i, j-1)$$

$$R_W \in I_E : \text{Motion to } (i+1, j)$$

$$R_W \in I_{\mathrm{NE}} : \text{Motion to } (i+1, j+1)$$

To terminate the random walk, first the parameter m_0 is defined as

$$m_0 = t/\Delta t \tag{14}$$

The random walk terminates after m_n number of steps when either of the two following cases occurs: 1) when the walker reaches an absorbing boundary (defined next) for $m_n < m_0$, or 2) when $m_n = m_0$.

In the first case the temperature of the boundary at time $(m_0 - m_n)\Delta t$ is registered as T_w, whereas in the second case the initial temperature of the final location (even if it is an interior node) is T_0 and registered as T_w. Repeating this procedure several times, the temperature of the specified location at time t can be calculated from Eq. (6).

IV. Treatment of Boundary Conditions

Treatment of the three common boundary condition types, that is, Dirichlet, Neumann, and Robin (convective), are discussed fully by Haji-Sheikh.[1] In this treatment the known temperature boundary (Dirichlet) is, so called, "fully absorbing," the convective is "partially absorbing," and the known heat-flux type (Neumann) boundary condition is "fully reflective." This latter implies that the random walk does not terminate when the walker reaches that boundary; instead, it is reflected back into the interior domain. In a fully absorbing boundary the walk is terminated at the boundary with the temperature of the boundary at the moment of the arrival of the walker registered as T_w. In a partially absorbing boundary condition absorption depends on the probability coefficients derived on the basis of the finite difference formulation of the differential equation.

V. Case Study

An example test case for unsteady anisotropic heat conduction is shown in Fig. 2. As shown in the figure, all of the boundaries are adiabatic (i.e., reflective) except for the one on the top, which is a convective boundary type with a convective heat-transfer coefficient h and the fluid temperature of T_∞ (i.e., a partially absorbing boundary). According to Fourier's law of heat conduction, the heat-flux components in an anisotropic material are given by

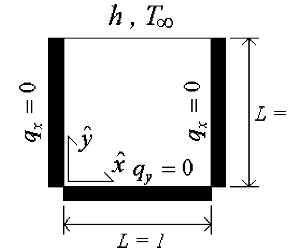

Fig. 2 Geometry and boundary conditions for the case under consideration.

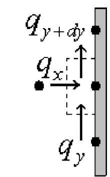

Fig. 3 Control volume for the right boundary.

$$q_x = -\left(k_{11}\frac{\partial T}{\partial x} + k_{12}\frac{\partial T}{\partial y}\right) \tag{15}$$

$$q_y = -\left(k_{12}\frac{\partial T}{\partial x} + k_{22}\frac{\partial T}{\partial y}\right) \tag{16}$$

Using control volumes similar to the one shown in Fig. 3, also using Eqs. (15) and (16), the conservation equations at the boundaries are obtained as follows:

Left boundary:

$$\hat{k}_{12}\frac{\partial^2 T}{\partial \hat{x}\partial \hat{y}} + \frac{\partial^2 T}{\partial \hat{y}^2} + \frac{2}{\Delta \hat{x}}\left(\frac{\partial T}{\partial \hat{x}} + \hat{k}_{12}\frac{\partial T}{\partial \hat{y}}\right) = \frac{1}{\alpha}\frac{\partial T}{\partial t} \tag{17}$$

Right boundary:

$$\hat{k}_{12}\frac{\partial^2 T}{\partial \hat{x}\partial \hat{y}} + \frac{\partial^2 T}{\partial \hat{y}^2} - \frac{2}{\Delta \hat{x}}\left(\frac{\partial T}{\partial \hat{x}} + \hat{k}_{12}\frac{\partial T}{\partial \hat{y}}\right) = \frac{1}{\alpha}\frac{\partial T}{\partial t} \tag{18}$$

Lower boundary:

$$\frac{\partial^2 T}{\partial \hat{x}^2} + \hat{k}_{12}\frac{\partial^2 T}{\partial \hat{x}\partial \hat{y}} + \frac{2}{\Delta \hat{y}}\left(\hat{k}_{12}\frac{\partial T}{\partial \hat{x}} + \frac{\partial T}{\partial \hat{y}}\right) = \frac{1}{\alpha}\frac{\partial T}{\partial t} \tag{19}$$

Upper boundary:

$$\frac{\partial^2 T}{\partial \hat{x}^2} + \hat{k}_{12}\frac{\partial^2 T}{\partial \hat{x}\partial \hat{y}} - \frac{2}{\Delta \hat{y}}\left(\hat{k}_{12}\frac{\partial T}{\partial \hat{x}} + \frac{\partial T}{\partial \hat{y}}\right) - \frac{2h}{\sqrt{k_0 k_{22}}\,\Delta \hat{y}}\left(T - T_\infty\right) = \frac{1}{\alpha}\frac{\partial T}{\partial t} \tag{20}$$

Discretizing the preceding equations with $\Delta \hat{x} = \Delta \hat{y}$, and reducing them to the form given by Eq. (7), the probability coefficients for each boundary type can be determined. Results are summarized in Tables 2 and 3, respectively, for surface and corner boundaries. More details are given by Irano.[10]

The parameters $\hat{h}$ and F in Tables 2 and 3 are given by

$$\hat{h} = h\Big/\sqrt{k_0 k_{22}} \tag{21}$$

$$F = \alpha \Delta t\Big/\Delta \hat{x}^2 \tag{22}$$

As can be seen in Tables 2 and 3, the summation of the probability coefficients is equal to one for each case, and none of coefficients is negative. Hence, according to the random walk algorithm, as the walker reaches the lower, right, or left boundaries he is redirected back into the domain. However, when the walker reaches the upper

Table 2 Probability coefficients for surface boundary nodes

Coefficient	Left	Right	Lower	Upper
P_0	$\hat{k}_{12}F - 4F + 1$	$\hat{k}_{12}F - 4F + 1$	$\hat{k}_{12}F - 4F + 1$	$\hat{k}_{12}F - 4F + 1 - 2\hat{h}F\Delta\hat{x}$
P_N	F	$F(1-\hat{k}_{12})$	$F(2-\hat{k}_{12})$	——
P_E	$F(2-\hat{k}_{12})$	——	F	$F(1-\hat{k}_{12})$
P_S	$F(1-\hat{k}_{12})$	F	——	$F(2-\hat{k}_{12})$
P_W	——	$F(2-\hat{k}_{12})$	$F(1-\hat{k}_{12})$	F
P_{NE}	$\hat{k}_{12}F$	——	$\hat{k}_{12}F$	——
P_{SW}	——	$\hat{k}_{12}F$	——	$\hat{k}_{12}F$
P_∞	——	——	——	$2\hat{h}F\Delta\hat{x}$

Table 3 Probability coefficients for corner boundary nodes

Coefficient	Left-down	Right-down	Left-up	Right-up
P_0	$1-4F-4\hat{k}_{12}F$	$1-4F-4\hat{k}_{12}F$	$1-4F+4\hat{k}_{12}F-2\hat{h}F\Delta\hat{x}$	$1-4F-4\hat{k}_{12}F-2\hat{h}F\Delta\hat{x}$
P_N	$2F(1+\hat{k}_{12})$	$2F(1-\hat{k}_{12})$	——	——
P_E	$2F(1+\hat{k}_{12})$	——	$2F(1-\hat{k}_{12})$	——
P_S	——	——	$2F(1-\hat{k}_{12})$	$2F(1+\hat{k}_{12})$
P_W	——	$2F(1-\hat{k}_{12})$	——	$2F(1+\hat{k}_{12})$
P_∞	——	——	$2\hat{h}F\Delta\hat{x}$	$2\hat{h}F\Delta\hat{x}$

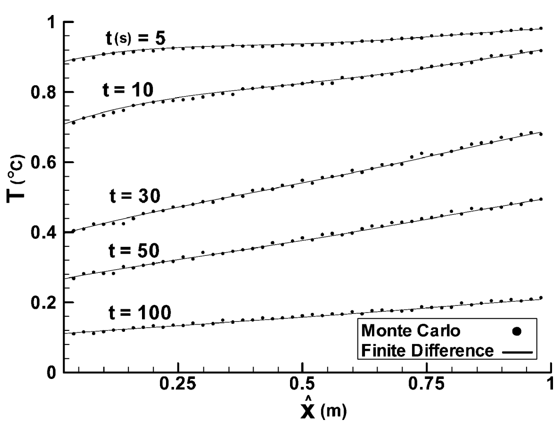

Fig. 4 Temperature distribution in $\hat{y} = 0.5$.

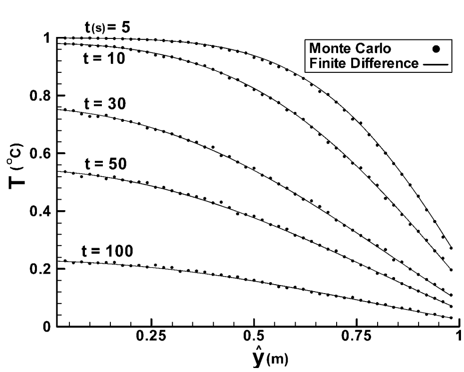

Fig. 5 Temperature distribution in $\hat{x} = 0.5$.

boundary (the partially absorbing boundary), depending on the value of the drawn random number R_w, the walk can be terminated and the fluid temperature T_∞ be registered as T_w for, or the walk can be carried on by redirecting the walker into the domain. The former occurs when $R_w < P_\infty$, whereas the latter occurs otherwise.

VI. Results

Figures 4 and 5 present the temperature distributions, respectively, on midplanes $\hat{x} = 0.5$ and $\hat{y} = 0.5$ obtained by the fixed-step random walk procedure.

To obtain these results, a network of 50×50, uniformly spaced, grid points was used with 10,000 trips initiating from each point whose temperature is to be determined. Values of heat-conduction parameters were set at $\hat{k}_{12} = 0.5$, $\alpha = 0.01$, and $\hat{h} = 10$. The fluid and initial temperatures were, respectively, set at $T_\infty = 0$, $T_0 = 1$. The time step used for computations was $\Delta t = 0.01$ s.

In the absence of a known exact analytical solution for this problem, the finite difference method with an identical grid network was used for validation of results. Although no concrete statement can be made regarding the accuracy of the Monte Carlo method, as the finite difference method cannot be considered exact, results obtained by the two methods compare to within 1% of each other on the average (globally in space and time). The relative sample variance of the error for all results obtained by the Monte Carlo method in this work is on the order of 6×10^{-5}. These results indicate that the same degree of confidence can be awarded to the Monte Carlo method as for the finite difference method for cases similar as the one considered in this work.

VII. Conclusions

The fixed-step random walk algorithm was successfully implemented for calculation of the temperature field in a general anisotropic medium. For the test case considered results compare very well with those obtained by the finite difference method.

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