CONDITIONS FOR THE COMPATIBILITY OF PROCESSES INVOLVING MOBILE INTERFACES AND THE STEFAN PROBLEM

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The nature of the Hadamard algorithm is analyzed, and a simple method is outlined for constructing the Hadamard and Predvoditelev algorithms. Generalized conditions which hold at interfaces in transport problems are found.

We assume two regions separated by some surface f(x, y, z, t) = 0, and we assume that the transport of some scalar Γ (temperature, concentration, etc.) satisfies the following equation within each of the adjacent regions:

$$L_i(\Gamma) = 0, \; i = 1, \; 2, \tag{1}$$

where the operator L_i has the same structure for both regions, but not at the interface, at which a conversion may occur on one side. In this case we have

$$L_1 = \Psi(\Gamma_1); \quad L_2 = \Psi(\Gamma_2) + \gamma \frac{\partial m}{\partial t}, \tag{2}$$

where γ is the conversion constant. In general, the operators L_i may have various structures, e.g., in the case in which there are sources distributed throughout the volume, in the case of convective forces, etc.

If these equations are to have single-valued solutions, and if the boundary motion itself is to be unidirectional, this motion must satisfy compatibility conditions. Some quantitative relations reflecting these conditions were derived by Hugoniot [1] and Hadamard [2] for shock waves.

Turning to the compatibility conditions for transport processes describable by the operators

$$\Psi(\Gamma_i) = \frac{\partial \Gamma_i}{\partial t} - \varkappa_i \Delta \Gamma_i = 0, \tag{3}$$

we find

$$\delta \frac{\partial \Gamma}{\partial t} = \delta [\varkappa \Delta \Gamma], \; x = \xi, \tag{4}$$

which we can replace in certain cases by the equivalent

$$\frac{\partial}{\partial t} \delta \Gamma = \frac{\partial}{\partial x} \delta \left[\varkappa \frac{\partial \Gamma}{\partial x} \right], \quad x = \xi. \tag{5}$$

Since the front moves as a result of the conversion (the primary equation) and the transport (the secondary equations), the integrals Γ_i(x, y, z, t) contain wave solutions.* We can thus write the latter relation in terms of the characteristic ξ = V(x, y, z) + gt, where V(x, y, z) is the equation of the front surface; and g

*As was first pointed out by A. S. Predvoditelev.

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the wave velocity:

$$\frac{\partial\,\delta\Gamma}{\partial\xi}\frac{d\xi}{dt}=\frac{\partial}{\partial\xi}\,\delta\left(\varkappa\frac{\partial\Gamma}{\partial x}\right)\frac{\partial V}{\partial x},\qquad x=\xi. \tag{6}$$

For the one-dimensional case we have V = x and thus ∂V/∂x = 1; it follows from (6) that

$$\delta\Gamma\frac{d\xi}{dt}\Big|_{\xi_0}^{\xi}-\int_{\xi_0}^{\xi}\delta\Gamma\,d\left(\frac{d\xi}{dt}\right)=\delta\left(\varkappa\frac{\partial\Gamma}{\partial x}\right)\Big|_{\xi_0}^{\xi}. \tag{7}$$

It follows that if the discontinuity $\delta\Gamma$ is equal to zero or some other constant, the discontinuity in the flux of this quantity at the interface is equal to zero or some other constant. It follows that, with the initial discontinuity in Γ, Eq. (7) is a condition on the coordinate of the interface.

We now assume that a source of intensity $\psi(x, y, z, t)$ is acting at the interface; then we replace (5) by

$$\frac{\partial}{\partial t}\delta\Gamma=\frac{\partial}{\partial x}\left[\varkappa\frac{\partial\Gamma}{\partial x}\right]+\psi(t),\quad x=\xi: \tag{8}$$

finding

$$\delta\Gamma\frac{d\xi}{dt}\Big|_{t_0}^{t}-\int_{t_0}^{t}\left[\delta\Gamma\left(\frac{d^2\xi}{dt^2}\right)+\psi(t)\frac{d\xi}{dt}\right]dt=\left[\delta\left(\varkappa\frac{\partial\Gamma}{\partial x}\right)\right]_{t_0}^{t}.\qquad x=\xi. \tag{9}$$

It is easy to see that this generalized relation includes the Stefan condition as a particular case.

We first consider the case in which we have a superheating or supercooling $\delta\Gamma$ = const ≠ 0 at the interface. In this case we have

$$-\int_{t_0}^{t}\psi(t)\frac{d\xi}{dt}dt=\left[\delta\left(\varkappa\frac{\partial\Gamma}{\partial x}\right)\right]_{t_0}^{t},\qquad x=\xi\,. \tag{10}$$

If

$$\left|\left[\delta\left(\varkappa\frac{\partial\Gamma}{\partial x}\right)\right]_{t_0}^{t}\right|\gg\left|\int_{t_0}^{t}v(t)\,d\left(\frac{d\xi}{dt}\right)\right|, \tag{11}$$

i.e., if the heat flux is sufficient so that the latent heat does not suppress solidification at the front surface (the case of the heat problem), we have the Stefan condition

$$-v(t)\frac{d\xi}{dt}\Big|_{t_0}^{t}=\left[\delta\left(\varkappa\frac{\partial\Gamma}{\partial x}\right)\right]_{t_0}^{t}, \tag{12}$$

where

$$v(t)=v(0)+\int_0^t\psi(t)\,dt. \tag{13}$$

The physical meaning of (11) is that the front acceleration is negligibly low. This inequality holds whenever we have $\xi \sim t$, at large t, with $\xi \sim \sqrt{t}$, and in many other cases. This analysis also holds for the case $\delta\Gamma = 0$.

Under these assumptions, the Stefan problem can be used to determine the coordinate of the front.

The Hadamard procedure is based on the assumption $\delta\Gamma$ = const, of which a particular case is $\delta\Gamma = 0$. Generalized relations (9) above are based on the assumption that operators δ and ∂ commute, although they contain more information than could be obtained by applying only the Hadamard algorithm to the problem. There is yet another way to generalize the Hadamard algorithm, suggested by Professor A. S. Predvoditelev [3].

In this paper we will generalize the Hadamard algorithm in a manner slightly different from that of [3].

We assume

$$\delta\Gamma = X(t). \tag{14}$$

Then the following equations must be compatible:

$$\begin{gathered} \frac{\partial f}{\partial x}dx + \frac{\partial f}{\partial y}dy + \frac{\partial f}{\partial z}dz = 0, \\ \left(\frac{\partial}{\partial x}\delta\Gamma - \frac{\partial X}{\partial x}\right)dx + \left(\frac{\partial}{\partial y}\delta\Gamma - \frac{\partial X}{\partial y}\right)dy + \left(\frac{\partial}{\partial z}\delta\Gamma - \frac{\partial X}{\partial z}\right)dz = 0. \end{gathered} \tag{15}$$

Hence we have

$$\frac{\partial}{\partial x_i}(\delta\Gamma - X) = \bar{\lambda}_1 \frac{\partial f}{\partial x_i}; \quad x_1 = x,\ x_2 = y,\ x_3 = z. \tag{16}$$

If we assume that only operators d and δ commute, we find

$$\sum \delta\left(\frac{\partial\Gamma}{\partial x_i}dx_i\right) = \sum \frac{\partial X}{\partial x_i}dx_i, \tag{17}$$

or, since dx_i is not varied, and the variation is independent of df,

$$\delta\frac{\partial\Gamma}{\partial x_i} = \frac{\partial X}{\partial x_i}. \tag{18}$$

We thus have

$$\delta\frac{\partial\Gamma}{\partial x_i} = -\bar{\lambda}_1\frac{\partial f}{\partial x_i} + \frac{\partial}{\partial x_i}\delta\Gamma. \tag{19}$$

This is the generalized algorithm for the discontinuity in the first derivative. Replacing Γ by the derivative $\partial\Gamma/\partial x_i$, we find

$$\begin{gathered} \delta\frac{\partial^2\Gamma}{\partial x_i^2} = -\lambda'\frac{\partial f}{\partial x_i} + \frac{\partial}{\partial x_i}\delta\frac{\partial\Gamma}{\partial x_i} = -\lambda'\frac{\partial f}{\partial x_i} \\ + \frac{\partial}{\partial x_i}\left[-\bar{\lambda}_1\frac{\partial f}{\partial x_i} + \frac{\partial}{\partial x_i}\delta\Gamma\right] = -\left(\frac{\partial\bar{\lambda}_1}{\partial x_i} + \lambda'\right)\frac{\partial f}{\partial x_i} - \bar{\lambda}_1\frac{\partial^2 f}{\partial x_i^2} + \frac{\partial^2}{\partial x_i^2}\delta\Gamma. \end{gathered} \tag{20}$$

This is the generalized algorithm for a discontinuity in the second derivative. For a mixed derivative we have

$$\delta\frac{\partial^2\Gamma}{\partial x_i\,\partial x_i} = -\lambda''\frac{\partial f}{\partial x_i} + \frac{\partial}{\partial x_i}\left[-\bar{\lambda}_1\frac{\partial f}{\partial x_j} + \frac{\partial}{\partial x_j}\delta\Gamma\right] = -\lambda''\frac{\partial f}{\partial x_i} - \frac{\partial\bar{\lambda}_1}{\partial x_i}\frac{\partial f}{\partial x_j} - \bar{\lambda}_1\frac{\partial^2 f}{\partial x_i\partial x_j} + \frac{\partial^2\delta\Gamma}{\partial x_i\partial x_j}. \tag{21}$$

Hence, writing [3]

$$-\lambda^u = \frac{\lambda_2}{H_f^2}\frac{\partial f}{\partial x_j} = -\lambda'\frac{\frac{\partial f}{\partial x_j}}{\frac{\partial f}{\partial x_i}} \quad \text{and} \quad -\bar{\lambda}_1 = \frac{\lambda_1}{H_f}, \tag{22}$$

we find the generalized Predvoditelev algorithm

$$\delta\frac{\partial^2\Gamma}{\partial x_i\partial x_j} = \left[\frac{\lambda_2}{H_f^2} + \frac{d}{df}\left(\frac{\lambda_1}{H_f}\right)\right]\frac{\partial f}{\partial x_i}\frac{\partial f}{\partial x_j} + \frac{\lambda_1}{H_f}\frac{\partial^2 f}{\partial x_i\partial x_j} + \frac{\partial^2\delta\Gamma}{\partial x_i\partial x_j}. \tag{23}$$

We thus see that the Predvoditelev algorithms are consequences of the commutation of d and δ. Obviously, other generalizations of the algorithms are possible for discontinuities in the derivatives.

We will now use a generalized Predvoditelev algorithm to write the conditions characterizing the motion of an interface between media. For this purpose we write the right and left sides of the equation

$$\delta \frac{\partial \Gamma}{\partial t} - \psi(t) = a\delta\left(\frac{\partial^2 \Gamma}{\partial x_i^2}\right) \tag{24}$$

as

$$\delta \frac{\partial \Gamma}{\partial t} - \psi(t) = \delta \frac{\partial \Gamma}{\partial t} - \gamma \frac{\partial m}{\partial t} = \delta \frac{\partial \Gamma}{\partial t} - \gamma \frac{\partial m}{\partial \Gamma} \frac{\partial \Gamma}{\partial t}$$

$$= \left[\frac{\lambda_1}{H_f} \frac{\partial f}{\partial t} + \frac{\partial}{\partial t} \delta\Gamma - \gamma \frac{\partial m}{\partial \Gamma} \frac{\partial \Gamma}{\partial t}\right] = -\left[\frac{\lambda_1}{H_f} + \frac{\partial \delta\Gamma}{\partial \xi} - \gamma \frac{\partial m}{\partial \xi}\right] g_\xi H_V \tag{25}$$

and

$$a\delta\left(\frac{\partial^2 \Gamma}{\partial x_i^2}\right) = a\left\{\left[\frac{\lambda_2}{H_f^2} + \frac{d}{d\xi}\left(\frac{\lambda_1}{H_f}\right)\right] H_V^2 + \frac{\lambda_1}{H_V} \nabla^2 V + H_V^2 \frac{\partial^2 \delta\Gamma}{\partial \xi^2}\right\}, \quad H_f = H_V. \tag{26}$$

We thus find the interface velocity to be

$$g_\xi = \frac{d\xi}{dt} = \frac{-a\left\{\left[\frac{\lambda_2}{H_V^2} + \frac{d}{d\xi}\left(\frac{\lambda_1}{H_V}\right)\right] H_V^2 + \frac{\lambda_1}{H_V} \nabla^2 V + H_V^2 \frac{\partial^2 \delta\Gamma}{\partial \xi^2}\right\}}{H_V\left[\frac{\lambda_1}{H_V} + \frac{\partial \delta\Gamma}{\partial \xi} - \gamma \frac{\partial m}{\partial \xi}\right]}. \tag{27}$$

When it is necessary to take into account a discontinuity in the first derivative $\partial\Gamma/\partial x_i$, we find

$$g_\xi = -\frac{\frac{a\lambda_2}{H_V^2} + \frac{\partial}{\partial \xi} \delta\left(a \frac{\partial \Gamma}{\partial x_i}\right)}{\frac{\lambda_1}{H_V} + \frac{\partial \delta\Gamma}{\partial \xi} - \gamma \frac{\partial m}{\partial \xi}}. \tag{28}$$

Comparing this expression with that found from (6), we see that in the generalized Predvoditelev algorithm there are additional terms with derivatives of the corresponding discontinuities. To study these terms, we write the discontinuity operation in the following symbolic form:

$$\delta \frac{\partial \Gamma}{\partial x_i} = \frac{(\delta \partial)\Gamma}{\partial x_i} + \frac{\partial(\delta\Gamma)}{\partial x_i} = \frac{\delta^* \Gamma}{\partial f} \frac{\partial f}{\partial x_i} + \frac{\partial(\delta\Gamma)}{\partial x_i} = -\bar{\lambda}_1 \frac{\partial f}{\partial x_i} + \frac{\partial(\delta\Gamma)}{\partial x_i} = \frac{\lambda_1}{H_f} \frac{\partial f}{\partial x_i} + \frac{\partial(\delta\Gamma)}{\partial x_i}, \tag{29}$$

$$\delta \frac{\partial \Gamma}{\partial t} = \frac{(\delta \partial)\Gamma}{\partial t} + \frac{\partial(\delta\Gamma)}{\partial t} = \frac{\delta^* \Gamma}{\partial f} \frac{\partial f}{\partial t} + \frac{\partial(\delta\Gamma)}{\partial t} = \frac{\lambda_1}{H_f} \frac{\partial f}{\partial t} + \frac{\partial(\delta\Gamma)}{\partial t}. \tag{30}$$

Here the operation δ^*/∂ denotes the conditional derivative of a function for the case in which the discontinuity of this function is not constant. If this discontinuity is equal to zero or some other constant, we have $\delta^* = \delta\partial$. The conditional derivative vanishes if the operations δ and ∂ are interchangeable; this result means that the parameter of a first-order discontinuity vanishes. The condition that operations δ and ∂ be interchangeable thus implies the independence of Γ from f.

We turn now to a discontinuity of the second derivative:

$$\delta\left(\frac{\partial^2 \Gamma}{\partial x_i \partial x_j}\right) = \frac{\delta^*}{\partial f}\left(\frac{\partial \Gamma}{\partial f}\right) \cdot \frac{\partial f}{\partial x_i} \frac{\partial f}{\partial x_j} + \frac{\partial}{\partial x_i}\left(\delta \frac{\partial \Gamma}{\partial x_j}\right) = \frac{\lambda_2}{H_f^2} \frac{\partial f}{\partial x_i} \frac{\partial f}{\partial x_j} + \frac{\partial}{\partial x_i}\left(\delta \frac{\partial \Gamma}{\partial x_j}\right), \tag{31}$$

where x_i and x_j are the spatial coordinates and the time. It follows that commutation of δ and ∂ implies the independence of $\partial\Gamma/\partial f$ from f. In this case the parameter for a second-order discontinuity vanishes.

Similarly, we can introduce the parameter of a discontinuity of order n,

$$\frac{\delta^*}{\partial f}\left(\frac{\partial^{n-1} \Gamma}{\partial f^{n-1}}\right) = \frac{\lambda_n}{H_f^n} \tag{32}$$

and we can generalize the algorithm,

$$\delta\left(\frac{\partial^n \Gamma}{\partial x_1 \partial x_2 \dots \partial x_n}\right) = \frac{\delta^*}{\partial f}\left(\frac{\partial^{n-1}\Gamma}{\partial f^{n-1}}\right)\frac{\partial f}{\partial x_1}\cdot\frac{\partial f}{\partial x_2}\dots\frac{\partial f}{\partial x_n}$$

$$+\frac{\partial}{\partial x_1}\left(\delta\frac{\partial^{n-1}\Gamma}{\partial x_2 \dots \partial x_n}\right) = \frac{\lambda_n}{H_f^n}\frac{\partial f}{\partial x_1}\dots\frac{\partial f}{\partial x_n} + \frac{\partial}{\partial x_1}\left(\delta\frac{\partial^{n-1}\Gamma}{\partial x_2 \dots \partial x_n}\right). \tag{33}$$

We now list the three algorithms under consideration here:

1. The Generalized Predvoditelev Algorithm. This algorithm is based only on the commutation of operators δ and d. The discontinuities of the function itself and of its derivatives are assumed not equal to zero or other constants.

2. The Hadamard Algorithm. This algorithm is also based on the commutation of operators d and δ, but it is based on the assumption that the discontinuities of the function vanish [2] but that those of the derivatives do not (see n° 72 in [2] and n° 74). This algorithm is a particular case of the Predvoditelev algorithm.

3. The Algorithm Based on the Commutation of δ and ∂ as well as on that of δ and d. This algorithm is based on the assumption that the function Γ and its derivatives along the surface are independent of the surface itself; by "independent" here we mean that there is no conditional derivative of these functions along the surface.

In connection with these results, we quote Hadamard [4]: "As yet no meaning has been found for a discontinuity of infinite order, i.e., one for which the types of motion must be treated as different, even though the partial derivatives of any order of the unknown function remain continuous at the wave."

If the basic partial differential equation contained derivatives with respect to the coordinates of order higher than in (3), e.g., of order n, then the numerator in (28) would contain discontinuity parameters of up to n-th order and derivatives with respect to ξ of the discontinuities in the (n − 1)th derivatives. If we now set all the discontinuities in such an expression equal to zero, the interface could still move. Moreover, if we set $\partial m/\partial \xi = 0$ in such an expression the interface velocity would become

$$g_\xi = \frac{aH_V}{\lambda_1}\sum_{l=2}^{n}\frac{\lambda_l}{H_V^l}. \tag{34}$$

As an example we will apply the symbolic method to the equation describing diffusion in accordance with the generalized equation

$$\sum_{n=1}^{N_1}\frac{\tau^n}{n!}\frac{\partial^n C}{\partial t^n} = \alpha\sum\frac{h^n}{n!}\frac{\partial^n C}{\partial x^n}. \tag{35}$$

We find

$$\sum_{n=1}^{N_1}\frac{\tau^n}{n!}\left[\frac{\lambda_n}{H_f^n}\left(\frac{\partial f}{\partial t}\right)^n + \frac{\partial}{\partial t}\left(\delta\frac{\partial^{n-1}C}{\partial t^{n-1}}\right)\right] = \alpha\sum_{n=1}^{N_2}\left[\frac{h^n}{n!}\frac{\lambda_n}{H_f^n}\left(\frac{\partial f}{\partial x}\right)^n + \frac{\partial}{\partial x}\left(\delta\frac{\partial^{n-1}C}{\partial x^{n-1}}\right)\right] + \psi(t), \tag{36}$$

where ψ(t) denotes the source function at the interface. Here the discontinuities in the derivatives with respect to the spatial coordinates can be reduced by the procedure above to a discontinuity in the function itself. With a known Γ(t) at the interface, the problem of finding the coordinate of the moving interface is ultimately solved outside the framework of the boundary-value problem.

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