SOME FEATURES OF THE VARIATIONAL FORMULATION OF THE GENERAL CRITERION OF EVOLUTION IN THE LOCAL POTENTIAL METHOD

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The variational formulation of nonlinear problems of the thermodynamics of irreversible processes in the local potential method is subjected to a comparative analysis. The particular example of the solution obtained by the method of successive approximations is examined and the possibility of using other methods is discussed.

The local potential method, proposed by Prigogine, Glansdorff, and Hays [1], is one of the possible attempts to apply the general criterion of evolution [2] to the variational formulation of nonlinear problems of the thermodynamics of irreversible processes. The starting premises are the existence of local equilibrium in some region of the system and the satisfaction of Onsager's symmetry relations for the phenomenological coefficients in the stationary state. In the local potential method the phenomenological coefficients are not assumed constant and hence, in principle, the method is applicable to any nonequilibrium stationary problem satisfying the above-mentioned starting premises.

The local potential is the rate of entropy production in which the true phenomenological coefficients L_{ij}, relating the thermodynamic fluxes J_i and the thermal forces X_j,

$$J_i = \sum_j L_{ij} X_j \,, \tag{1}$$

are replaced by their values L_{ij}^0 in the stationary state. Thus, the local potential

$$P = \int_V dV \sum_i \sum_j L_{ij}^0 X_i X_j \tag{2}$$

in the stationary state itself coincides with the rate of entropy production, while near the stationary state the rate of variation of local potential with time satisfies* the general criterion of evolution

$$\dot{P} = 2 \int_V dV \sum_i \sum_j L_{ij}^0 X_i \dot{X}_j \leqslant 0. \tag{3}$$

From the definition of the local potential it is clear that it is an extremal function of state only in the stationary state itself, while in the neighborhood of the stationary state, not being a function of state, it can only decrease with time. This property makes it possible to formulate a variational principle analogous to the theorem of minimum rate of entropy production:

$$\delta P = 0, \quad \delta^2 P > 0 \tag{4}$$

for the nonlinear region of the phenomenological relations.

To formulate the variational principle it is usually more convenient to characterize the state of the system not with respect to the forces X_i, but with respect to certain functions of the forces $Z_s(X_i)$, which completely determine the state and hence X_i. Thus, in problems of heat conduction it is more convenient to find the distribution of the temperature itself and not the gradient of its reciprocal. In this case the steady state will correspond to functions Z_s^0 and hence

$$L_{ij}^0 = L_{ij}(Z_s^0). \tag{5}$$

With this in mind, we can formulate variational problem (4) in general form as the problem of finding m unknown functions $Z_s(q_k)$ $(s = 1, 2, \ldots, m)$, defined in the closed fixed region V of the space of generalized coordinates q_k $(k = 1, 2, \ldots, l)$ satisfying the boundary conditions

$$G_p(q_k;\ Z_s;\ (Z_s)'_{q_k}) = 0 \quad (p = 1, 2, \ldots, m) \text{ on } \Sigma \tag{6}$$

and minimizing the functional

$$P(Z_s) = \int \sum_{i=1}^{n} \sum_{j=1}^{n} L_{ij}(Z_s^0;\ (Z_s^0)'_{q_k})\, X_j(Z_s;$$

$$(Z_s)'_{q_k})\, X_i(Z_s, (Z_s)'_{q_k})\, dq \quad (dq = dq_1 dq_2 \ldots dq_l) \tag{7}$$

with the additional condition

$$Z_s^0(q_k) = Z_s(q_k) \quad (s = 1, 2, \ldots, m). \tag{8}$$

A feature of variational problem (6), (7), (8) is the dependence of the integrand function—the Lagrangian $\mathscr{L}$ of the functional P— on the two sets of functions Z_s and Z_s^0, the variation being carried out only with respect to the Z_s, whereas the Z_s^0 are assumed known; in fact, the functions Z_s^0 are not known, since they represent the unknown solution. The significance of this will be evident from an examination of the Euler Equations.

The extremum condition is written as follows:

$$\delta P = \int_V \left\{ \sum_{s=1}^{m} \left[\frac{\partial \mathscr{L}}{\partial Z_s^0} - \sum_{k=1}^{l} \left(\frac{\partial \mathscr{L}}{\partial (Z_s^0)'_{q_k}} \right)'_{q_k} \right] \delta Z_s^0 + \right.$$

$$\left. + \sum_{s=1}^{m} \left[\frac{\partial \mathscr{L}}{\partial Z_s} - \sum_{k=1}^{l} \left(\frac{\partial \mathscr{L}}{\partial (Z_s)'_{q_k}} \right)'_{q_k} \right] \delta Z_s \right\} dV = 0. \tag{9}$$

* The criterion of evolution asserts the nonpositiveness of the form

$$\int_V dV \sum_i \sum_j L_{ij} X_i \dot{X}_j,$$

which differs from (3) by quantities of the next order of smallness.

Since the functions Z_s^0 are assumed known, $\delta Z_s^0 = 0$, and in view of the arbitrariness of δZ_s, we obtain the Euler equations

$$\frac{\partial \mathscr{L}}{\partial Z_s} - \sum_{k=1}^{l} \left[\frac{\partial \mathscr{L}}{\partial (Z_s)'_{q_k}} \right]'_{q_k} = 0. \quad (10)$$

We denote the product $X_i X_j$ by X_{ij}. Then the Langrangian $\mathscr{L}$ will have the form

$$\mathscr{L} = \sum_i^n \sum_j^n L_{ij} (Z_s^0, (Z_s^0)'_{q_k}) X_{ij} (Z_s, (Z_s)'_{q_k}), \quad (11)$$

and the Euler equations are represented by

$$\sum_i^n \sum_j^n \left[L_{ij} \frac{\partial X_{ij}}{\partial Z_s} - \sum_k^l \frac{\partial}{\partial q_k} \left(L_{ij} \frac{\partial X_{ij}}{\partial (Z_s)'_{q_k}} \right) \right] =$$
$$= \sum_i \sum_j \left[L_{ij} \frac{\partial X_{ij}}{\partial Z_s} - \sum_k^l \left(\frac{\partial L_{ij}}{\partial q_k} \frac{\partial X_{ij}}{\partial (Z_s)'_{q_k}} + \right. \right.$$
$$\left. \left. + L_{ij} \frac{\partial}{\partial q_k} \frac{\partial X_{ij}}{\partial (Z_s)'_{q_k}} \right) \right] = 0, \quad (12)$$

where

$$\frac{\partial L_{ij}}{\partial q_k} = \sum_{t=1}^m \left[\frac{\partial L_{ij}}{\partial Z_t^0} (Z_t^0)'_{q_k} + \sum_{p=1}^l \frac{\partial L_{ij}}{\partial (Z_t^0)'_{q_p}} (Z_t^0)''_{q_p q_k} \right],$$

$$\frac{\partial}{\partial q_k} \frac{\partial X_{ij}}{\partial (Z_s)'_{q_k}} = \sum_{t=1}^m \left[\frac{\partial^2 X_{ij}}{\partial (Z_s)'_{q_k} \partial Z_t} (Z_k)'_{q_k} + \right.$$
$$\left. + \sum_{p=1}^l \frac{\partial^2 X_{ij}}{\partial (Z_s)'_{q_k} \partial (Z_t)'_{q_p}} (Z_t)''_{q_p q_k} \right].$$

Taking condition (8) into account, we obtain

$$\sum_{i,j}^n \sum_t^m \sum_{k,p}^l \left\{ (Z_t)''_{q_p q_k} \left[\frac{\partial L_{ij}}{\partial (Z_t)'_{q_p}} \frac{\partial X_{ij}}{\partial (Z_s)'_{q_k}} + \right. \right.$$
$$\left. + L_{ij} \frac{\partial^2 X_{ij}}{\partial (Z_t)'_{q_p} \partial (Z_s)'_{q_k}} \right] +$$
$$+ (Z_t)'_{q_k} \left[\frac{\partial L_{ij}}{\partial Z_t} \frac{\partial X_{ij}}{\partial (Z_s)'_{q_k}} + L_{ij} \frac{\partial^2 X_{ij}}{\partial Z_t \partial (Z_s)'_{q_k}} \right] -$$
$$\left. - L_{ij} \frac{\partial X_{ij}}{\partial Z_s} \right\} = 0. \quad (13)$$

The solution of this system of equations with boundary conditions (6) gives the unknown functions Z_s.

Here, as distinct from ordinary variational problem, there are two conditions: the functions Z_s^0 are assumed known $\delta Z_s^0 = 0$ and, moreover, equal to Z_s ($Z_s = Z_s^0$). To illustrate the significance of these two conditions we will sucessively discard them.

We start by discarding the first condition. Equation (9) will again be the condition of the extremum of the functional. Using condition (8), we reduce Eq. (9) to the form

$$\delta P = \int_V \sum_{s=1}^m \left[\frac{\partial \mathscr{L}}{\partial Z_s} - \sum_{k=1}^l \left(\frac{\partial \mathscr{L}}{\partial (Z_s)'_{q_k}} \right)'_{q_k} \right] \delta Z_s dV =$$
$$= 0. \quad (14)$$

Hence by virtue of the arbitrariness of δZ_s^0 we obtain the usual Euler equations in the form

$$\sum_{i,j}^n \left[\frac{\partial L_{ij}}{\partial Z_s} X_{ij} + L_{ij} \frac{\partial X_{ij}}{\partial Z_s} - \right.$$
$$\left. - \sum_{k=1}^l \frac{\partial}{\partial q_k} \left(\frac{\partial L_{ij}}{\partial (Z_s)'_{q_k}} X_{ij} + L_{ij} \frac{\partial X_{ij}}{\partial (Z_s)'_{q_k}} \right) \right] =$$
$$= 0. \quad (15)$$

Comparing (15) with (13), we obtain the identity conditions for these equations,

$$\sum_{i,j}^n \left[\frac{\partial L_{ij}}{\partial Z_s} X_{ij} - \sum_{k=1}^l \frac{\partial}{\partial q_k} \left(\frac{\partial L_{ij}}{\partial (Z_s)'_{q_k}} X_{ij} \right) \right] =$$
$$= 0. \quad (16)$$

These conditions can be satisfied for arbitrary X_{ij} only when L_{ij}, i.e., in the linear region of the phenomenological relations. Thus, discarding the condition $\delta Z_s^0 = 0$ leads to the theorem of minimum entropy production.

We now discard the second condition $Z_s = Z_s^0$. Equations (10), (11), (12) remain valid, but Eqs. (13) are not satisfied. In this case the final equations will be Eqs. (12), which for some choice of Z_s^0 again become ordinary Euler equations. Equations (12) serve for determining the next approximation. Hence discarding the condition $Z_s = Z_s^0$ leads to the method of successive approximations.

As an illustration of these general ideas we will consider the problem of nonlinear heat conduction in a solid.

In this case the general criterion of evolution is expressed through the known condition of thermodynamic stability. In fact, multiplying both sides of the equation of energy conservation

$$\rho \frac{\partial e}{\partial t} = - \operatorname{div} \mathbf{W} \quad (17)$$

by $\partial T^{-1}/\partial t$, we obtain

$$\rho \frac{\partial T^{-1}}{\partial t} \frac{\partial e}{\partial t} = - \rho \frac{c_V}{T^2} \left(\frac{\partial T}{\partial t} \right)^2 \leqslant 0, \quad (18)$$

since the specific heat is positive definite. Hence for the right side there also follows

$$- \frac{\partial T^{-1}}{\partial t} \operatorname{div} \mathbf{W} =$$
$$= - \operatorname{div} \left(\frac{\partial T^{-1}}{\partial t} \mathbf{W} \right) + \mathbf{W} \operatorname{grad} \frac{\partial T^{-1}}{\partial t} \leqslant 0. \quad (19)$$

Integrating over the volume and applying the Ostrogradskii-Gauss formula, we obtain the inequality

$$-\int_{\Sigma} \mathbf{W} \frac{\partial T^{-1}}{\partial t} d\vec{\sigma} + \int_{V} \mathbf{W} \frac{\partial}{\partial t} \operatorname{grad} T^{-1} dV \leqslant 0. \quad (20)$$

For stationary boundary conditions the first integral is equal to zero. Thus,

$$\int_{V} \mathbf{W} \frac{\partial}{\partial t} \operatorname{grad} T^{-1} dV \leqslant 0, \quad (21)$$

which is also the expression for general criterion of evolution in the given case. The equality corresponds to the stationary state.

We use Fourier's law with temperature-dependent thermal conductivity λ:

$$\mathbf{W} = -\lambda(T) \operatorname{grad} T = \lambda(T) T^2 \operatorname{grad}(T^{-1}). \quad (22)$$

Then

$$\int_{V} \lambda(T) T^2 \operatorname{grad} T^{-1} \frac{\partial}{\partial t} \operatorname{grad} T^{-1} dV = \frac{1}{2} \int_{V} \lambda(T) T^2 \frac{\partial}{\partial t} (\operatorname{grad} T^{-1})^2 dV \leqslant 0. \quad (23)$$

In order to obtain an expression for the local potential, we substitute for the phenomenological coefficient L its value in the stationary state L^0, i.e., instead of $\lambda(T)T^2$ we write $\lambda(T_0)T_0^2$, where T_0 is the stationary temperature distribution. Then, as in the general case (3),

$$\frac{\partial}{\partial t} \int_{V} \lambda(T_0) T_0^2 (\operatorname{grad} T^{-1})^2 dV = \frac{\partial P}{\partial t} \leqslant 0. \quad (24)$$

Hence there follows the variational problem: to find the temperature distribution satisfying certain boundary conditions and minimizing the functional

$$P = \int_{V} \lambda(T_0) T_0^2 (\operatorname{grad} T^{-1})^2 dV \quad (25)$$

with the additional condition $T = T_0$.

We write the Euler equation for this problem. Taking into account the condition of fixed stationary distribution,

$$\delta T_0 = 0, \quad (26)$$

we obtain the equation

$$-4 \frac{\lambda T_0^2}{T^5} (\operatorname{grad} T)^2 - \operatorname{div}\left(2 \frac{\lambda T_0^2}{T^4} \operatorname{grad} T\right) = -4 \frac{\lambda T_0^2}{T^5} (\operatorname{grad} T)^2 - 2\left(\frac{\lambda' T_0^2 + 2\lambda T_0}{T^4}\right) \operatorname{grad} T_0 \operatorname{grad} T + 8 \frac{\lambda T_0^2}{T^5} (\operatorname{grad} T)^2 - 2 \frac{\lambda T_0^2}{T^4} \Delta T = 0, \quad (27)$$

hence, using the condition $T_0 = T$, we obtain the stationary equation of heat conduction

$$\lambda \Delta T + \lambda_T' (\operatorname{grad} T)^2 = 0, \quad (28)$$

which represents Eq. (13) for the case of heat conduction.

Finally, we discard the fixity condition (26). Then the Lagrangian

$$\mathscr{L} = \lambda(T) T^2 (\operatorname{grad} T^{-1})^2 = \lambda(T) T^{-2} (\operatorname{grad} T)^2, \quad (29)$$

and the Euler equation takes the form

$$(\lambda' T^{-2} - 2\lambda T^{-3}) (\operatorname{grad} T)^2 - \operatorname{div}(2\lambda T^{-2} \operatorname{grad} T) = \frac{2}{T^2}\left(\frac{\lambda'}{2} - \frac{\lambda}{T}\right)(\operatorname{grad} T)^2 - \frac{4}{T^2} \times \left(\frac{\lambda'}{2} - \frac{\lambda}{T}\right)(\operatorname{grad} T)^2 - \frac{2\lambda \Delta T}{T^2} = 0, \quad (30)$$

whence follows the equation

$$\lambda \Delta T + \lambda_T' (\operatorname{grad} T)^2 = \left(\frac{\lambda}{T} + \frac{\lambda_T'}{2}\right)(\operatorname{grad} T)^2. \quad (31)$$

This equation goes over into the stationary equation of heat conduction when the right side is equal to zero, i.e., when one of the following two conditions is satisfied: $\lambda/T + \lambda_T'/2 = 0$, whence $\lambda(T) = cT^{-2}$, or $(\operatorname{grad} T)^2 = 0$, whence T = const. Obviously, these are precisely the cases when L = const, i.e., when the stationary state lies in the linear region of the phenomenological relations.

In this case the general equation (12) is represented by Eq. (27), which can be used to determine the next approximation to the stationary temperature distribution in the method of successive approximations.

APPENDIX

We will compare the temperature distributions given by the local potential method, the theorem of minimum entropy production and the method of successive approximations for the problem of nonlinear heat conduction.

We will consider a heat-conducting segment of length l, at whose ends the temperature values T_1 and T_2 are given. Introducing the dimensionless variables $x = x_{\text{dim}}/l$ and $T = T_{\text{dim}}/T_1$ and assuming, to be specific, $T_2 = 2T_1$, we obtain the boundary conditions of the problem in the form

$$T(0) = 1, \quad T(1) = 2. \quad (1^*)$$

We also assume a linear law of variation of the thermal conductivity

$$\lambda(T) = \lambda_0 (1 + \alpha T), \quad (2^*)$$

where λ_0 and α are certain constants.

For this special case the stationary equation of heat conduction (28) is written in the form

$$(1 + \alpha T) T_{xx}'' + \alpha (T_x')^2 = 0. \quad (3^*)$$

It is easy to verify that the solutions of this equation are

$$T = -1/\alpha + \sqrt{c_1 x + c_2} \text{ when } \alpha \neq 0,$$

$$T = c_3 x + c_4 \text{ when } \alpha = 0, \qquad (4^*)$$

where the values of the constants are found from boundary conditions (1*).

Solutions (4*) give the actual stationary temperature distributions for various values of α obtained by the local potential method.

For this case Eq. (31) is expressed as follows:

$$[TT''_{xx} - (T'_x)^2] + \alpha T \left[TT''_{xx} - \frac{1}{2}(T'_x)^2\right] = 0. \qquad (5^*)$$

For comparison with the exact solution (4*) we will consider the same limiting values $\alpha = 0$ and $\alpha = \infty$. Obviously, at these values of the parameter α the form of the solution will be as follows:

$$T = c_1 \exp(c_2 x) \quad \text{when } \alpha = 0,$$

$$T = c_3 x^2 + c_4 x + \frac{c_4^2}{4c_3} \text{ when } \alpha = \infty, \qquad (6^*)$$

where the values of the constants are again easily found from boundary conditions (1*). Solutions (6*) are the distributions corresponding to minimization of entropy production, and not local potential, i.e., these distributions are obtained as a result of applying the methods of ordinary thermodynamics of irreversible quasi-equilibrium processes.

$$T_0(1 + \alpha T_0)\,[2(T'_x)^2 - TT''_{xx}] - TT'_x T'_{0x}(2 + \alpha T_0) = 0. \qquad (7^*)$$

We start by selecting as the zero approximation T_0 that for which L = const, i.e., T_0 = const. Then for all values of α Eq. (7*) gives a solution of the form

$$T = c_1 (x + c_2)^{-1}. \qquad (8^*)$$

If as the zero approximation we take $T_0 = 1 + x$, which corresponds to the stationary temperature distribution at $\lambda(T)$ = const, the form of the solution will be different:

$$T = c_3 [(1 + x)^{-2} + c_4]^{-1} \text{ when } \alpha = \infty,$$

$$T = c_5 x + c_6 \text{ when } \alpha = 0. \qquad (9^*)$$

A comparison with the exact solution compels us to give preference to the starting approximation $\lambda(T)$ = = const.

For comparison we write the stationary temperature distributions obtained, using (1*),

by the local potential method

$$T = 1 + x \text{ when } \alpha = 0,$$

$$T = \sqrt{3x + 1} \text{ when } \alpha = \infty, \qquad (10^*)$$

by the method based on application of the theorem of minimum entropy production

$$T = 2^x \text{ when } \alpha = 0,$$

$$T = (3 - 2\sqrt{2})\,x^2 + (2\sqrt{2} - 2)\,x + 1 \text{ when } \alpha = \infty, \qquad (11^*)$$

and by the method of successive approximations

$$T = \frac{2}{2 - x} \text{ when } L = \text{const and for any } \alpha,$$

$$T = 1 + x \text{ when } T_0 = 1 + x \text{ and } \alpha = 0,$$

$$T = 3\left[1 - \frac{2}{(1 + x)^2 + 2}\right] \text{ when } T_0 = 1 + x,$$

$$\text{while } \alpha = \infty.$$

NOTATION

J_i is the thermodynamic flux; X_i is the thermodynamic force; L_{ij} is the phenomenological coefficient; ρ is the density; e is the energy per unit mass; W is the heat flux; V is the volume of the system; Σ is the boundary surface; $d\vec{\sigma}$ is the element of the boundary surface; $\lambda(T)$ is the temperature-dependent thermal conductivity.

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