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ON THE SEARCH FOR VARIATIONAL PRINCIPLES

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Abstract—Several attempts to formulate variational principles for non-self-adjoint and nonlinear systems are examined. The variational formulations are found to lack the advantages of genuine variational principles, chiefly because the variational integral is not stationary or because no variational integral exists. The corresponding variational methods of approximation are shown to be equivalent to the more straightforward Galerkin method or another closely related version of method of weighted residuals. The methods due to Rosen (restricted variations), Glansdorff and Prigogine (local potential), and Biot (Lagrangian thermodynamics) are treated. It is concluded that there is no practical need for variational formulations of the sort examined.

NOMENCLATURE

a_i, functions of time in a trial solution;
A, Hamiltonian in equations (3) and (4), Onsager's functional in equations (21–28);
$\mathbf{A}$, acceleration in equation (18), arbitrary vector field in equation (67);
$\mathbf{A}_k$, acceleration of k^{th} particle;
C_v, heat capacity per unit mass at constant volume;
$\hat{\delta D}$, functional of infinitesimal magnitude, defined in equation (70);
$\hat{\delta D}_s$, functional of infinitesimal magnitude, defined in equation (70);
f, function;
$\mathbf{f}_i$, function;
F, function;
$\mathbf{F}$, force;
$\mathbf{F}_k$, force on k^{th} particle;
$\mathbf{F}'_k$, force on k^{th} particle not derivable from a potential;
g, function;
h, Biot's so-called total heat, defined by equation (64);
h_s, heat-transfer coefficient on boundary;
$\mathbf{H}$, Biot's so-called heat-flow vector, defined by equation (67);
J_2, functional defined by equation (19);
$\hat{\delta J}$, functional of infinitesimal magnitude defined by equation (17);
J_n, normal flux $\mathbf{n} \cdot \mathbf{J}$;
$\mathbf{J}$, flux vector;
k, thermal conductivity;
K, linear differential operator;
L, Lagrangian in equation (2), linear differential operator elsewhere;
L^*, adjoint operator;
L_{gg}, phenomenological coefficient in equations (31–33);
m_k, mass of k^{th} particle;
MWR, method of weighted residuals;
$\mathbf{n}$, outward pointing unit normal;
N, number of adjustable parameters;
$P(\ )$, bilinear concomitant, defined by equation (10);
$q_i(t)$, adjustable functions of time in trial solution;
$\dot{q}_i(t)$, time derivatives of q_i;
Q_i^*, Biot's so-called generalized thermal force, defined in equation (81);
$\mathbf{R}_k$, position of k^{th} particle;
$\mathfrak{R}$, thermal conductivity dyadic;
S, boundary (surface) of system;
$\dot{S}$, rate of entropy accumulation within volume;
$\dot{S}^*$, rate of entropy outflow from surface;
t, time;

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$\mathbf{t}$, traction;
T, kinetic energy in equation (2), temperature elsewhere;
$\mathfrak{T}$, stress;
u, function;
$\mathbf{u}$, material velocity;
$\mathfrak{U}$, idemfactor;
V, potential energy in equation (2), Biot's so-called thermal potential in equation (68) *et seq.*, interior (volume) of system elsewhere;
$\widehat{\delta W}$, virtual work, defined in equation (1);
$\mathbf{x}$, position;
y, alias variable;
Y, alias variable;
Z, alias variable.

Greek symbols

α, functions of time in a trial solution;
α_i, adjustable constants in a trial solution;
β_i, adjustable constants in a trial solution;
δ, variation operator (subscript denotes what is held fixed during variation);
∇, gradient operator;
ϵ, infinitesimally small parameter;
ρ, density;
ϕ, function;
Φ, rate of entropy production in equations (21–22); functional elsewhere;
ψ, function.

Subscripts

s, surface quantity;
0, alias variable.

Superscripts

*, trial solution.

1. INTRODUCTION

A VARIATIONAL description of a physical system consists of a statement that the variation, or functional differential, of a specified functional is equal to some fixed value, which can be and customarily is chosen to be zero. The description is not complete without full specification of (i) the functions with respect to which the variation, or differential, is taken, and (ii) any auxiliary conditions that must be satisfied as constraints when the variation is taken. The functional whose variation vanishes is said to be stationary relative to (i) those functions with respect to which the variation is taken, and (ii) any constraints that are imposed. The stationary property of an integral functional implies by the calculus of variations one or more "Euler equations" and "natural boundary and initial conditions." If these match the equations of change, constitutive equations, boundary conditions, and so on, which describe the physical behavior of the system, then the variational formulation is indeed an alternative description. This type of stand-in is commonly called a *variational principle*, although seldom in a physical or any other sense is it an ultimate basis; it is no more a principle than any other equally accurate mathematical description of the performance of the same physical system.

In some instances the varied functional is not merely stationary but actually attains a local maximum or minimum. The variational principle can then be stated as a superlative—some function of the behavior of the system is greatest, or least, under certain constraints. This type of statement lends itself to teleological speculation and holds a singular appeal for many minds as the history of variational principles in dynamics and quantum mechanics testifies [50; compare 24 and 32]. Indeed, some statements that in fact involve no more than a stationary functional are habitually referred to as "minimum principles," Hamilton's principle and the principle of least action being the most famous cases in point. It appears that the special appeal of superlatives has inspired a significant part of the search for variational principles in areas outside dynamics.

A variational formulation may be useful in summarizing a subject and it may, as Morse and Feshbach [34] remark, suggest fruitful analogies and generalizations. In dynamics, for example,

it may be advantageous to introduce postulates about material interactions via a potential, Lagrangian, or Hamiltonian function rather than as the equivalent constitutive relation for the force of interaction. The same authors [34] remark that in the development of a subject, the differential equations (by which they mean equations of change, constitutive equations, and so forth—not necessarily in the form of differential equations) have generally been worked out first and only later have equivalent variational formulations been found. This is certainly the pattern in the areas discussed below. Regarding the area of classical mechanics, Goldstein's comment [24] bears repeating:

> It has been pointed out that variational principles in themselves contain no new physical content, and they rarely simplify the practical solution of a given mechanical problem. Their value lies chiefly as starting points for new formulations of the theoretical structure of classical mechanics. For this purpose Hamilton's principle is especially fruitful, and to a lesser extent, so also is the principle of least action. The others have proved to be of little use, except as they have led to fruitless teleological speculations.

Much of the remark is equally true of variational principles in other fields.

A variational formulation leads to the so-called variational method of obtaining approximate solutions to the problem of predicting system performance. The method consists of substituting in the stationary functional a trial solution containing a number of adjustable parameters; the functional is varied with respect to these parameters, which are then so evaluated as to make the variation vanish in accordance with the variational formulation. One of the main advantages of the variational method is that in the choice of functional form for the trial solution "it permits the exploitation of any information bearing on the problem such as might be available from purely intuitional consideration" [34] or from prior experience with related problems. Now this is also an outstanding advantage of direct approximating schemes such as the method of weighted residuals.

Indeed, the variational method shares this and some other advantages of the method of weighted residuals [10, 8, 16]. What has been overlooked in the search for variational principles is that whereas MWR—the method of weighted residuals—can be applied to any problem, whether or not it is linear and self-adjoint, the variational method is only applicable to those problems for which a variational principle exists and has been found, a common situation only when the system of equations is linear and self-adjoint. (A kind of variational formulation is possible for linear, non-self-adjoint systems and their adjoints together, as advocated by Morse and Feshbach [34, chapters 3 and 9]; the method of least squares also amounts to a variational formulation involving the adjoint, as shown by Mikhlin and discussed in the next section.) However, if a genuine variational principle is available it may provide advantages over MWR: (1) The variational integral may represent a physical quantity of more use for the needs at hand than the field given by the solution, and the variational method is likely to approximate this integral more accurately than it approximates the solution. (2) If the principle is a minimum or maximum principle, the variational method provides upper or lower bounds on the variational integral. (3) If in addition a reciprocal variational principle (maximum or minimum) can be formulated, both upper and lower bounds can be found, and these may be close enough together to have real utility. (4) The direct method of the calculus of variations may yield proof of existence of solutions, a potential advantage when an exhaustive study of the mathematical aspects of a problem seems indicated. In view of these advantages it is not surprising that much effort has been expended on the search for variational principles for nonlinear and non-self-adjoint systems.

Unfortunately, only relatively few classes of

physical systems can be represented by self-contained variational formulations, that is, without bringing in adjoint or "mirror-image" systems. And within each of these classes only a small proportion can be represented by minimum or maximum principles. From a pragmatic standpoint the main shortcoming of variational formulations is that the variational methods which they support provide no approximation scheme that cannot be set up more simply and more quickly as one of the standard direct approximating methods, in particular, one or another version of MWR. This criticism is elaborated below.

The whole subject is muddied by the overworking of the term, "variational principle," in the literature, where formulations that merely resemble classical variational formulations are also called variational principles, even though they are still farther from being basic physical principles in the usual sense. Examples occur in recent formulations known as restricted variational principles, one instance being the "Method of the Local Potential" put forward by Glansdorff and Prigogine, and in Biot's "Lagrangian Thermodynamics". All treat heat conduction and other transport phenomena and have roots in Onsager's 1931 variational formulation of Fourier's law of heat conduction, a constitutive relation. All of the formulations named here are taken up after a brief recapitulation of more conventional variational approaches in the next section.

Section 3 deals with approximation methods based on "restricted variations", which might equally well be called "partial functional differentials" or "infinitesimal functions" or "quasi-variational principles". It is shown that all of these methods lack the special advantages that are usually associated with variational principles. It is also shown that they are substantially equivalent to the more straightforward method of Galerkin, one version of MWR. In the final section it is concluded that the recent mutants are sterile, at least so far as generation of constitutive relations and practical calculations are concerned. The search for variational principles has been pushed too far.

2. VARIATIONAL FORMULATIONS

An oft-cited advantage of variational principles is that they provide concise statements of the physical principles which are reproduced by the Euler equations of the stationary functional. The leading examples are in the field of particle mechanics, which makes an excellent background for subsequent discussion.

D'Alembert's principle for any system of particles is stated in terms of infinitesimals called virtual displacements and virtual work [see, e.g. 29]: the total virtual work is zero for all admissible reversible displacements; i.e.

$$\bar{\delta W} \equiv \sum_{k=1}^{N} (\mathbf{F}_k - m_k \mathbf{A}_k) \cdot \delta \mathbf{R}_k = 0 \qquad (1)$$

where $\mathbf{F}_k$ is the net force on the k^{th} particle, which has mass m_k and suffers acceleration $\mathbf{A}_k$. The overbar on $\bar{\delta W}$ indicates that the total virtual work is a differential form which cannot be expressed as the variation of a scalar functional. Hamilton's principle corrects this deficiency by integrating virtual work over a definite time interval [29]:

$$\int_{t_1}^{t_2} \bar{\delta W}\, \mathrm{d}t \equiv \delta \int_{t_1}^{t_2} (T - V)\, \mathrm{d}t \equiv \delta \int_{t_1}^{t_2} L\, \mathrm{d}t \qquad (2)$$

where T is the total kinetic energy of the particles and V is the potential energy corresponding to the forces $\mathbf{F}_k$, which have to be conservative. The quantity $L \equiv T - V$ is the kinetic potential, or Lagrangian; its integral

$$A \equiv \int_{t_1}^{t_2} L\, \mathrm{d}t$$

is a functional of the coordinates which specify the configuration of the particles. This functional is stationary for all admissible variations of the coordinates as functions of time. Provided the functional form for the kinetic potential is known—which can only be so when the forces

are derivable from a potential—Hamilton's variational principle,

$$\delta A = 0, \qquad \delta A = \int_{t_1}^{t_2} \delta\hat{W}\, dt \tag{3}$$

always leads to the equations of particle motion. Consequently it is possible to derive equations of motion under various types of conservative forces by postulating different forms for the Lagrangian, L. This is no longer possible when some of the forces $\mathbf{F}_k'$, cannot be derived from a potential, in which case constitutive equations for them must be used. Retaining the form of Hamilton's principle one can write

$$\delta A + \sum_{k=1}^{N} \int_{t_1}^{t_2} \mathbf{F}_k' \cdot \delta\mathbf{R}_k\, dt = 0 \tag{4}$$

and call this a "variational principle". One can also retreat to d'Alembert's formulation, $\delta\hat{W} = 0$, perhaps calling even it a "variational principle". This usage is not in line with the classical mathematics of variations, because in both cases *there is no functional which is stationary.* The differential principles of mechanics—d'Alembert's, Gauss's, Hertz's, the above distention of Hamilton's—are not genuine variational principles, whereas Hamilton's and other stationary integral principles are; the latter are, as just indicated, of somewhat more restricted applicability. A similar situation occurs in the search for variational formulations for continuous systems.

Consider the type of boundary-value problem that describes steady-state behavior of many linear systems:

$$L[u(\mathbf{x})] = g(\mathbf{x}), \qquad \mathbf{x} \text{ in } V \tag{5}$$

$$u = f(\mathbf{x}), \qquad \mathbf{x} \text{ on } S \tag{6}$$

where L is a linear, differential operator and the boundary function is given. Is it possible to formulate a variational principle with equation (5) as its Euler equation?

It is always possible to write a "principle" of the form

$$\hat{\delta J} \equiv \int_v [L(u) - g]\, \delta u\, dV = 0 \tag{7}$$

which necessarily implies equation (5), $L(u) = g$ in V. But equation (7) embodies nothing more than the mere definition of an inexact functional differential: there may or may not exist a functional J which is stationary. If the problem is self-adjoint, however, such a functional does exist: it is

$$J \equiv \int_v [\tfrac{1}{2}L(u) - g]\, K(u)\, dV. \tag{8}$$

Its first variation with respect to admissible state-functions, u, is

$$\delta J = \int_v \tfrac{1}{2}L(\delta u)K(u)\, dV + \int_v [\tfrac{1}{2}L(u) - g]\, K(\delta u)\, dV \tag{9}$$

and, in virtue of the K-self-adjointness of the operator, L,

$$\int_v L(\delta u)\, K(u)\, dV = \int_v L(u)\, K(\delta u)\, dV + \int_v P(K; u, \delta u)\, dS. \tag{10}$$

Thus

$$\delta J = \int_v [L(u) - g]\, K(\delta u)\, dV \tag{11}$$

provided of course that an auxiliary, linear, homogenous operator, K, can be and has been so chosen that the bilinear concomitant, $P(K; u, \delta u)$, vanishes under the boundary conditions that are to be satisfied.† For self-adjoint problems, there always exists a functional which is stationary—virtually by definition. And for non-self-adjoint problems there is no variational formulation of the same sort, i.e. self-contained.

An analogy exists between the problem of finding a variational principle which has as its Euler equation a given differential equation and the problem of finding a scalar potential which has as its gradient a given vector. A vector

† The auxiliary operator is simply unity in the classical definition of self-adjointness [cf. 34]. The broader definition in terms of the K-adjoint encompasses any boundary conditions which have essentially self-adjoint nature that would otherwise not be apparent.

can be derived from a scalar potential only if it is irrotational, of course. The theory of gradient mappings teaches that a variational principle can be found for linear differential equations only if the operator is self adjoint [42].

In the case of linear problems that are not self-adjoint, it is possible to give a variational formulation for the original problem and its adjoint, or "mirror image", coupled inextricably together as a system of equations. This approach was advocated by Morse and Feshbach [34] and has been adopted on occasion [43, 45, 31]. The variational method to which it leads is an instance of the method of moments, a version of MWR closely related to the Galerkin method [13, 16]. The second alternative, in the case of linear differential systems, is to double the order of the differential equation by applying to it the adjoint operator. Thus, corresponding to equation (5), viz. $L(u) = g$, the following equation is self-adjoint, as may easily be verified:

$$L^*L(u) = L^*(g) \tag{12}$$

where L^* is the adjoint operator to L. Now Mikhlin [33] has shown that the classical variational formulation for this self-adjoint equation is equivalent to *minimizing* the positive definite integral

$$J \equiv \int_V [L(u) - g]^2 \, dV. \tag{13}$$

This functional of u measures the total squared residual by which the function fails to satisfy equation (5). Its minimization with respect to adjustable parameters in a trial solution—with due attention to boundary conditions and boundary residuals—is precisely the least-squares method, another special case of MWR.

Minimization of the total squared residual applies equally well to non-linear problems; as a variational principle it leads to the method of least squares as a variational method. In this light it has been advocated and tested by Becker [1]. But for problems of transient performance, linear and nonlinear alike, the least-squares technique has limited utility because each instant of time requires separate treatment [14, 16]. It is effective when the time course of the system is of less interest than its state at a particular instant in its evolution [1, chapter 4]. Thus, the class of nonlinear problems that can be given classical variational formulations, much less self-contained ones, is severely limited. Apart from isolated cases, e.g. discovery in a lone case of a "mirror system" analogous to the adjoint system [48, 17], the search for stationary functionals is fruitless.

In order to escape the impasse without abandoning variational formalism, various authors have simply adopted looser definitions of "variational principle." In their lexicon the term covers two formulations that are really equivalent. By way of illustrating these, consider the type of problem that describes transient performance of many linear systems:

$$L[u(\mathbf{x}, t)] = \frac{\partial u}{\partial t}, \qquad \mathbf{x} \text{ in } V, \qquad t > 0 \tag{14}$$

$$u = g(\mathbf{x}), \qquad \mathbf{x} \text{ in } V, \qquad t \leqslant 0 \tag{15}$$

$$u = f(\mathbf{x}, t), \qquad \mathbf{x} \text{ on } S, \qquad t > 0. \tag{16}$$

In the first approach one defines an inexact functional differential, or inexact variation, the vanishing of which implies the original equation:

$$\widehat{\delta J} \equiv \int_0^t \int_V \left[L(u) - \frac{\partial u}{\partial t} \right] \delta u \, dV \tag{17}$$

Not uncommonly integration over time is omitted, the infinitesimal δJ then being a function of time rather than a functional, and the infinitesimal δu having the significance of an instantaneous variation better represented by $\delta_t u$—matters that are outside the pale of classical variational calculus and go unexplained in formulations where they are important. Whether or not integration over time is performed, the characteristic feature of this scheme is that no functional J exists whose variation with respect to u has the form of equation (17). Because any advantages of a true variational principle are therefore absent, this type of formulation will be called a *quasi-variational principle*. The need for

such a term seems to have gone unfelt. For example, the following has been called a variational principle for fluid flow [46]:

$$\int_v \rho(\mathbf{F} - \mathbf{A}) \cdot \delta\mathbf{x}\, dV - \int_v \mathfrak{T} : \nabla\delta\mathbf{x}\, dV + \int_s \mathbf{t} \cdot \delta\mathbf{x}\, dS = 0 \qquad (18)$$

for all virtual displacements, $\delta\mathbf{x}$, which satisfy the kinematical conditions. (The acceleration $\mathbf{A}$, body-force $\mathbf{F}$, stress tensor $\mathfrak{T}$, surface traction $\mathbf{t}$, and density ρ are all functions of position, $\mathbf{x}$, and time.) As Serrin [46] pointed out, "The reader will observe that . . . [this] variational principle is little more than a reformulation of the equations of motion . . .".

The second approach stems from the idea of defining a functional of the state u and its rate of change $\partial u/\partial t$ as independent functions and then introducing a partial functional differential, or "restricted variation". Generally, however, integration over time is omitted and one works with an integral that remains a function of time. For example, when L is a self-adjoint spatial operator, the formalism can run

$$J(t) \equiv \int_v [\tfrac{1}{2}L(u) - y]\, u\, dV \qquad y = \frac{\partial u}{\partial t} \qquad (19)$$

$$\delta_y J \equiv \int_v [L(u) - y]\, \delta u\, dV = 0 \qquad (20)$$

the latter then implying equation (14).† The resemblance to classical calculus of variations is superficial, even when this scheme is employed for steady-state, non-self-adjoint, boundary-value problems. The most lucid advocate of this approach in the literature seems to have been Rosen [39, 41], who called it a *restricted variational principle*. The characteristic feature of this type of formulation is the presence of "alias variables" (y for $\partial u/\partial t$ above) which though held fixed during the variation have to be unmasked immediately after the variation is performed. As a result the variational integral is not stationary, and other advantages of true variational principles are lost as well. The situation is summarized in Table 1.

While both of these approaches retain some variational formalism and are called here *ad hoc* variational principles, the variational method of approximation to which they lead is indistinguishable from the Galerkin method applied to the original equations unadorned, as demonstrated by several cases about to be taken up. This equivalence is portrayed in Fig. 1. The question, then, is whether the variational formalism confers any advantage whatsoever. It is known that where a true variational principle

Table 1. Comparison of ad hoc variational formulations with variational principles

Property	Quasi-variational formulation	Restricted variational principle	Classical variational principle
Applicable to nonlinear and non-self-adjoint problems	Yes	Yes	Rarely
Variational integral exists and is defined†	No	Yes	Yes
Integral is stationary in calculations†	No	No	Yes
Requires explicit knowledge of basic equations *a priori*	Yes	Yes	Not necessarily
May be a minimum (or maximum) principle	No	No	Sometimes
May provide upper and lower bounds on variational integral or eigenvalue	No	No	Occasionally

† For cases in which all three formulations pertain.

† The subscript on the variation symbol δ indicates what field is to be held fixed in a restricted variation.

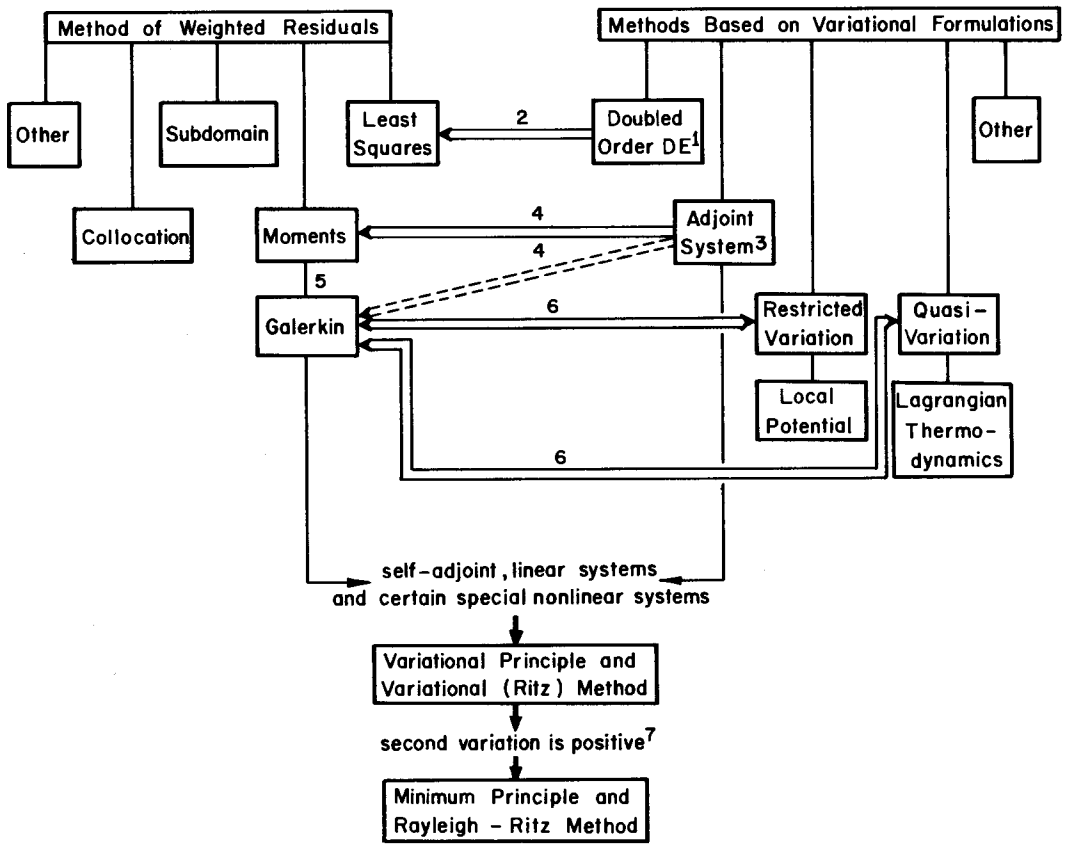

FIG. 1. Interrelationships of approximation methods for differential systems.
(1) Applicable only to linear equations. (2) Equivalence shown by Mikhlin [33]. (3) Applicable to all linear equations as well as certain special nonlinear equations. (4) Equivalence discussed in [13, 16]. (5) In method of moments the weighting functions are not the same functions used in the trial solution, whereas in the Galerkin method they are. (6) Equivalence shown below and in [14, 15]. (7) Additional conditions must be satisfied to insure the existence of a minimizing function.

exists, Ritz's method [8] based on the stationary integral is equivalent to Galerkin's method [8, 10]; and when there is a minimum principle, the Rayleigh-Ritz and Galerkin methods are equivalent [12, 10, 47]. In the latter circumstance blind use of the Galerkin procedure would overlook the fact that any trial solution yields an upper bound on the variational integral—which may be an eigenvalue or other quantity of greater interest than the solution; this fact is of course obvious in the variational formulation on which the Rayleigh–Ritz procedure rests. So when a true minimum (or maximum) principle exists, variational formalism does reveal a feature that may be turned to advantage in practical calculations. There is, however, no such feature in the types of systems for which quasi-variational and restricted variational formulations have been devised.

3. RESTRICTED VARIATIONS

By introducing partial functional differentials, or restricted variations, Rosen [39, 41], Glansdorff and Prigogine [22], and others have

formulated so-called variational principles. These are examined critically here. In each case, the variational method based on the restricted variational formulation turns out to be either Galerkin's method or a substantially equivalent version of the method of moments. The "variational principles" are then examined for any distinctive and redeeming advantages. The discussion begins with a review of Onsager's "variation principle" because this early example seems to have inspired many of the *ad hoc* variational formulations that are extant and forms the starting point for some of them.

For heat conduction in anisotropic media Onsager [35] formulated a variational principle that requires the fundamental equation of change and the particular constitutive equations to be clearly separated. His principle is that for certain simple materials the following integral of the heat flux and temperature fields

$$A(\mathbf{J}, T) \equiv \dot{S}(\mathbf{J}) + \dot{S}^*(J_n) - \phi(\mathbf{J}, \mathbf{J}) \quad (21)$$

is a maximum with respect to variations of the heat flux $\mathbf{J}$ under what he called the "convention" that the temperature distribution T is prescribed, i.e. the temperature field is already a known function of position (dependence on time is not discussed). A functional for systems in steady states, $A(\mathbf{J}, T)$ remains a function of time for transient systems. Its three parts are rate of entropy accumulation, outflow, and generation, respectively:

$$\left.\begin{aligned} \dot{S}(\mathbf{J}) \equiv -\int_v \frac{\nabla \cdot \mathbf{J}}{T}\,\mathrm{d}V, \dot{S}^*(J_n) \equiv \int_s \frac{\mathbf{n} \cdot \mathbf{J}}{T}\,\mathrm{d}S, \\ \Phi(\mathbf{J}, \mathbf{J}) \equiv \int_v \frac{\mathbf{J} \cdot \mathfrak{R} \cdot \mathbf{J}}{2T}\,\mathrm{d}V \end{aligned}\right\} \quad (22)$$

where $\mathfrak{R}$ is a known symmetric dyadic that may depend on temperature but not on heat flux. Accordingly

$$A(\mathbf{J}, T) = \int_v \mathbf{J} \cdot \left[\nabla\left(\frac{1}{T}\right) - \frac{\mathfrak{R} \cdot \mathbf{J}}{2T}\right]\mathrm{d}V \quad (23)$$

and the partial functional differential of $A(\mathbf{J}, T)$ with respect to $\mathbf{J}$ while holding the function T fixed is

$$\delta_T A = \int_v \delta\mathbf{J} \cdot \left[\nabla\left(\frac{1}{T}\right) - \frac{\mathfrak{R} \cdot \mathbf{J}}{T}\right]\mathrm{d}V. \quad (24)$$

For this partial variation to vanish the "Euler equation" is the constitutive relation generally known as Fourier's law for anisotropic media:

$$-\frac{1}{T}\nabla T = \mathfrak{R} \cdot \mathbf{J}. \quad (25)$$

In the well-known case of isotropic media, for which $\mathfrak{R} = \mathfrak{U}k/T$ ($\mathfrak{U}$ is the idemfactor), this of course reduces to the familiar form of Fourier's law:

$$\mathbf{J} = -k\nabla T. \quad (26)$$

The functional $A(\mathbf{J}, T)$ is a maximum so far as *partial* variations with respect to $\mathbf{J}$ are concerned because

$$\delta_T(\delta_T A) = -\int_v \frac{1}{T}\delta\mathbf{J} \cdot \mathfrak{R} \cdot \delta\mathbf{J}\,\mathrm{d}V \leqslant 0 \quad (27)$$

($\mathfrak{R}$ is presumed to be positive definite; T is absolute temperature).

It is perfectly clear that Onsager's variational formulation merely reproduces a particular constitutive equation for heat flux—Fourier's law—provided the temperature field is already known. The formulation just as clearly is *not* a maximum principle, or a genuine variational principle at all, when the temperature field is unknown, because then

$$\left.\begin{aligned} \delta A = \delta_J A + \delta_T, A, \\ \delta^2 A = \delta_J(\delta_J A) + \delta_J(\delta_T A) + \delta_T(\delta_J A) \\ + \delta_T(\delta_T A). \end{aligned}\right\} \quad (28)$$

The partial variation of A with respect to T does not vanish in general. Moreover, the negative signature of $\delta_T(\delta_T A)$ by no means implies a maximum principle. Onsager himself did not consider the real problem of calculating heat conduction phenomena. These are points neglected by later authors who have attempted to

develop a practicable variational method based on an extension of Onsager's formulation.

Rosen [39] showed that variational formalism can be manipulated to give somewhat different restricted variational principles of the same sort as Onsager's. Thus, for transient heat conduction in isotropic media he makes the integral $\int(\mathbf{J} \cdot \mathbf{J}/2k)\mathrm{d}V$ stationary with respect to variations in $\mathbf{J}$ subject to overwhelming constrains: (i) $\nabla \cdot \mathbf{J} + \rho C_v \partial T/\partial t = 0$, the equation of change; (ii) $\mathbf{n} \cdot \mathbf{J}$ is specified on the surface S; (iii) k is independent of $\mathbf{J}$; and (iv) both T and $\partial T/\partial t$ are known and held fixed throughout the region V. The Euler equation is just the constitutive relation, $\mathbf{J} = k\nabla T$. This is certainly one of the most elaborate representations of Fourier's law to be found anywhere. Rosen went on to formulate what he called a more useful variational principle which, unlike Onsager's, reproduces the full equation of change with Fourier's law:

$$\delta_Y \int_v \left[\rho C_v T Y + \frac{k}{2}(\nabla T)^2\right] \mathrm{d}V = 0, \qquad Y \text{ fixed}; \tag{29}$$

$$T \text{ specified on } S;$$

$$Y = \partial T/\partial t \text{ after variation};$$

this set of requirements yields the familiar differential equation,

$$\rho C_v \frac{\partial T}{\partial t} = \nabla \cdot (k \nabla T). \tag{30}$$

Rosen also discussed the variational method corresponding to (29). The temperature field is approximated by the finite sum, $T^* = \sum a_i(t) f_i(x)$, the functions $f_i(x)$ being a prescribed set, and the variation is carried out with the a_i as variables holding $\mathrm{d}a_i/\mathrm{d}t$ fixed. This strategem yields a set of ordinary differential equations for the $a_i(t)$ and is entirely equivalent to Galerkin's method, as has been shown [14].

Chambers [7] stated a similar formulation in which the temperature field is fixed while the variational integral is varied with respect to the time derivative, $\mathrm{d}a_i/\mathrm{d}t$. Herivel [26] attempted to formulate a restricted variational principle like Rosen's, though at first independently of the latter's. The variational integral and method of obtaining the correct "Euler equation" used by Hays [25] in following what is called the local potential method are precisely the same as Rosen's [39] for unsteady-state conduction with constant properties and vanishing heat flux on the boundary.

Later Rosen [40] showed how to develop a restricted variational principle for any differential equation by identifying the appropriate quantities to hold fixed during variation. As he found, it may be necessary to hold the very same quantity fixed at one place in the variational integral while allowing it to vary in others, a practice conveniently codified by giving the quantity an alias at one place or the other. His motivation was approximate solution of nonlinear differential equations by means of trial solutions with adjustable parameters. That the scheme flowing from his restricted variational principle is Galerkin's method and can be applied with no reference whatsoever to variational formalism has gone unremarked.

Still later Rosen [41] developed a restricted variational principle for unsteady-state problems in magnetohydrodynamics, with fluid properties that depend on the dependent variables. The variational integral depends on the state variable(s), say α, its time derivative $\dot{\alpha}$, and their appropriately chosen aliases, α' and $\dot{\alpha}'$. The integral $I(\alpha, \alpha', \dot{\alpha}')$ is varied with respect to α while holding α' and $\dot{\alpha}'$ fixed. Following this variation the aliases are removed by setting $\alpha' = \alpha$ and $\dot{\alpha}' = \dot{\alpha}$, thereby arriving at the correct "Euler equation". This procedure is precisely that used by Hays [25] in his application of the local potential method, an attempt to characterize stationary states of grossly nonequilibrium systems by something akin to minimum entropy production.

The so-called theorem of minimum entropy production as it is applied to steady-state heat

conduction with prescribed boundary temperature is [11]

$$\delta \int_v L_{gg} \left[\nabla\left(\frac{1}{T}\right)\right]^2 \mathrm{d}V = 0 \qquad (31)$$

for all variations in temperature which vanish on the boundary. If the phenomenological coefficient L_{gg} does not depend on temperature the Euler equation is

$$\nabla \cdot \left[L_{gg} \nabla\left(\frac{1}{T}\right)\right] = 0, \quad \text{or}$$

$$\nabla \cdot \left[\frac{L_{gg}}{T^2} \nabla T\right] = 0. \qquad (32)$$

If this is to be consistent with the heat-conduction equation it is necessary to make the identification

$$k = L_{gg}/T^2$$

$$\text{i.e.} \quad kT^2 = L_{gg} = \text{constant}. \qquad (33)$$

Requiring kT^2 to be constant is not realistic except for very nearly isothermal systems; indeed, the theorem of minimum entropy production applies only as an approximation to systems in steady state very close to equilibrium. Consequently many attempts [21, 18, 23] have been made to establish a more general minimum principle that reduces to the theorem of minimum entropy production in the neighbourhood of equilibrium. So far as steady-state heat conduction with temperature-independent conductivity and conventional boundary conditions is concerned the system is self-adjoint and there is no difficulty: Dirichlet's minimum principle and its modifications are well-known [see equation (40) below]. Even temperature-dependent conductivity can be handled despite its nonlinear character [15]. In any case the stationary functional is not the rate of entropy production and the formulation is equally applicable near and far from isothermal equilibrium.

But heat conduction is only one irreversible process. Recently Glansdorff and Prigogine [22] attempted a general variational description of irreversible processes by introducing what are named local potentials, ostensibly a generalization of entropy production. They state [22]:

> The main practical importance of these local potentials arises from the possibility of determining the stationary states through a variational principle.

The variational formulation by Glansdorff and Prigogine is not, despite claims to the contrary [22, 25, 19, 44] a minimum principle; it is not a classical variation principle but rather a restricted variational principle of the type treated by Rosen in 1954 [40]. The so-called self-consistent approximation scheme based on the local potential is the Galerkin method (or in some cases a closely related version of the method of moments). These features of Glansdorff–Prigogine local potential method have been illustrated with the case of steady-state heat conduction [15]; they have also been demonstrated in the case of the coupled Navier–Stokes and energy equations for steady states [13]. As an aid in evaluating it the method will be illustrated here with a simple example: unsteady-state heat conduction with Fourier's law as the constitutive relation heat flux, with temperature-dependent properties, and with Newton's law of cooling for the boundary condition (often called the linear radiation boundary condition). Apart from the boundary condition the same problem has been treated by Hays [25] following the local potential approach.

This example has the structure of equations (14–16) above; the equations are:

$$\rho C_v \frac{\partial T}{\partial t} - \nabla \cdot (k \nabla T) = 0 \quad \text{in} \quad V, \quad t > 0 \qquad (34)$$

$$k\mathbf{n} \cdot \nabla T + h_s(T - T_s) = 0 \quad \text{on} \quad S, \quad t > 0 \qquad (35)$$

$$T = \Psi(\mathbf{x}) \quad \text{in} \quad V, \quad t \leqslant 0. \qquad (36)$$

The initial temperature field Ψ and the external temperature distribution T_s are given. (The vector $\mathbf{n}$ is the outward pointing unit normal to the bounding surface S; ρ, C_v, k, and h_s are, of course, density, heat capacity, thermal

conductivity, and heat-transfer coefficient, respectively.) Suppose equations (34) and (35) are multiplied by an instantaneous variation of the temperature field that appears in them and integrated over the volume V and surface S, respectively; the results are†

$$\int_v \rho C_v \frac{\partial T}{\partial t} \delta_t T \, dV - \int_v \nabla . (k \nabla T) \delta_t T \, dV = 0 \quad (37)$$

$$\int_s k\mathbf{n} . \nabla T \, \delta_t T \, dS + \int_s h_s (T - T_s) \delta_t T \, dS = 0. \quad (38)$$

Rearrangement of equation (37) followed by application of the divergence theorem and addition of equation (38) yields the quasi-variational statement:

$$\int_v \tfrac{1}{2} k \delta_t (\nabla T)^2 \, dV + \int_v (\delta_t T) \rho C_v \frac{\partial T}{\partial t} dV + \int_S \tfrac{1}{2} h_s \delta_t (T - T_s)^2 \, dS = 0. \quad (39)$$

Although there is no functional being varied in equation (39), it does happen to reduce to the well-known variational principle for *steady-state conduction with temperature-insensitive k and h_s*:

$$\delta \Phi \equiv \delta \left[\tfrac{1}{2} \int_v k (\nabla T)^2 \, dV + \tfrac{1}{2} \int_S h_s (T - T_s)^2 \, dS \right] = 0. \quad (40)$$

For unsteady-state conduction with temperature-dependent k and h_s the quasi-variational statement can be converted to a restricted variational principle by introducing an alias $T_0(\mathbf{x}, t)$ for temperature and then setting

$$k = k_0 \equiv k(T_0), \qquad C_v = C_0 \equiv C_v(T_0),$$
$$\rho = \rho_0 \equiv \rho(T_0), \qquad h_s = h_0 \equiv h_s(T_0). \quad (41)$$

With $\partial T / \partial t$ temporarily replaced by $\partial T_0 / \partial t$, equation (39) is integrated over the time interval θ to t to give a functional of the two functions, T and T_0, which is the "local potential" for this problem:

$$\Phi[T, T_0] \equiv \int_\theta^t \int_v \left[\tfrac{1}{2} k_0 (\nabla T)^2 + \rho_0 C_0 T \frac{\partial T_0}{\partial t} \right] dV \, dt + \int_\theta^t \int_S \tfrac{1}{2} h_0 (T - T_s)^2 \, dS \, dt. \quad (42)$$

The restricted variational principle consists of requiring the local potential to be stationary with respect to variations of T with T_0 held fixed—and of course $\partial T_0 / \partial t$ as well. In symbols, $\delta_{T_0} \Phi[T, T_0] = 0$.

To show precisely what this means, let

$$\phi(\epsilon, \epsilon_0) \equiv \Phi[T + \epsilon Z, T_0 + \epsilon_0 Z_0]. \quad (43)$$

The total first variation of Φ is given by [9]

$$\delta \Phi \equiv \delta_{T_0} \Phi + \delta_T \Phi \equiv \epsilon \left(\frac{\partial \phi}{\partial \epsilon} \right)_{\epsilon = \epsilon_0 = 0} + \epsilon_0 \left(\frac{\partial \phi}{\partial \epsilon_0} \right)_{\epsilon = \epsilon_0 = 0} \quad (44)$$

In this case the total variation after rearranging and applying the divergence theorem takes the form

$$\begin{aligned} \delta \Phi = \epsilon \Bigg\{ & \int_\theta^t \int_v Z [\rho_0 C_0 \frac{\partial T_0}{\partial t} - \nabla . (k_0 \nabla T)] \, dV \, dt \\ & + \int_\theta^t \int_S Z [k_0 \mathbf{n} . \nabla T + h_0 (T - T_s)] \, dS \, dt \Bigg\} \\ & + \epsilon_0 \Bigg\{ \int_\theta^t \int_v Z_0 \left[\tfrac{1}{2} \frac{dk_0}{dT_0} (\nabla T)^2 \right. \\ & \left. + \frac{d(\rho_0 C_0)}{dT_0} T \frac{\partial T_0}{\partial t} - \frac{\partial}{\partial t} (\rho_0 C_0 T) \right] dV \, dt \\ & + \int_v [\rho_0 C_0 T Z_0]_\theta^t \, dV \\ & + \int_\theta^t \int_S Z_0 \left[\tfrac{1}{2} \frac{dh_0}{dT_0} (T - T_s)^2 \right] dS \, dt \Bigg\}. \end{aligned} \quad (45)$$

† In equations (37) and (38) the symbol $\delta_t T$ must be interpreted as standing for the product $\epsilon \eta(\mathbf{x})$ where $\eta(\mathbf{x})$ is an arbitrary function and ϵ is a small quantity independent of position, $\mathbf{x}$. This is an instantaneous variation, and both ϵ and $\eta(\mathbf{x})$ can be chosen differently at different instants of time. Compare the remark following equation (17).

For Φ to be stationary each of the sets of terms within square brackets must vanish; these requirements are the Euler equations and natural boundary conditions. After the alias for temperature is removed by invoking what Glansdorff and Prigogine call the subsidiary condition,

$$T = T_0, \quad \text{whence} \quad \epsilon = \epsilon_0 \quad \text{and} \quad Z = Z_0 \tag{46}$$

the Euler equations becomes

$$\rho C_v \frac{\partial T}{\partial t} - \nabla . (k \nabla T) = 0 \tag{34}$$

$$\tfrac{1}{2}\frac{\mathrm{d}k}{\mathrm{d}T}(\nabla T)^2 + \frac{\mathrm{d}(\rho C_v)}{\mathrm{d}T} T \frac{\delta T}{\partial t} - \frac{\delta(\rho C_v T)}{\partial t} = 0 \tag{47}$$

with natural boundary conditions

$$k\mathbf{n} . \nabla T + h_s(T - T_s) = 0 \tag{35}$$

$$\tfrac{1}{2}\frac{\mathrm{d}h_s}{\mathrm{d}T}(T - T_s)^2 = 0 \tag{48}$$

$$\rho C_v T = 0 \qquad \text{at} \quad t = t \tag{49}$$

and the essential condition

$$T = \Psi(\mathbf{x}) \qquad \text{at} \quad t = 0. \tag{36}$$

Now some of these equations occur as the original problem, but the solutions to that problem do not satisfy equations (47–49) and the local potential is not stationary—much less a minimum—with respect to variation of the temperature field from that which satisfies equations (34–36). While it is true that the second partial functional differential of the local potential, viz.

$$\delta_{T_0}(\delta_{T_0}\Phi) \equiv \epsilon^2 \left(\frac{\partial^2 \phi(\epsilon, \epsilon_0)}{\partial \epsilon^2}\right)_{\epsilon = \epsilon_0 = 0}$$

$$= \int_\theta^t \int_v k_0 (\nabla \delta T)^2 \, \mathrm{d}V \, \mathrm{d}t + \int_\theta^t \int_S h_0 (\delta T)^2 \, \mathrm{d}S \, \mathrm{d}t \tag{50}$$

is positive (provided $h_s \geqslant 0$) the total second functional differential $\delta^2\Phi$ is not necessarily positive (compare equation 28). Consequently, this does not imply a minimum principle by which an unknown solution to equations (34–36), which is to say *both* T and T_0, can be approximated.

Formally, the "Euler equation" and "natural boundary condition" for the restricted variational principle $\delta_{T_0}\Phi[T, T_0] = 0$ are

$$\rho_0 C_0 \frac{\partial T}{\partial t} - \nabla . (k_0 \nabla T) = 0 \tag{51}$$

$$k_0 \mathbf{n} . \nabla T + h_0(T - T_s) = 0. \tag{52}$$

When the alias for temperature is removed by recalling that $T_0 = T$, the original differential equation and boundary condition, equation (34) and (35) are recovered. Obviously this sort of variation formulation is fundamentally different from the classical type, in which the variation of a functional is taken with respect to all of the dependent variables.

An analogy in elementary calculus may further clarify the nature of the restricted variations employed by Rosen and Glansdorff and Prigogine. Consider the equation $g(x) = 0$ and let

$$f(x) = \int_c^x g(x') \, \mathrm{d}x'.$$

At one or more places in $f(x)$ replace the variable x by y, thereby generating a function of two variables, $f(x, y)$. The analog of a true variational principle for the solution of $g(x) = 0$ is the statement that $\mathrm{d}f(x, x)/\mathrm{d}x = 0$, i.e. that the value of x must make $f(x)$ stationary. In other words, the directional derivative of $f(x, y)$ in the direction $y = x$ must vanish at a point on the line $y = x$, as occurs at C in Fig. 2. One can easily verify that for this to happen it is necessary that $\partial f/\partial x = -\partial f/\partial y$ at the point in question. Contrast the analog of a restricted variational principle, which is constructed by introducing the alias variable in the original equation to generate $g(x, y) = 0$, and then integrating with respect to x alone to produce

$$f(x, y) = \int_c^x g(x', y) \, \mathrm{d}x';$$

the solution to the original equation corresponds now to the statement that $\partial f(x, y)/\partial x = 0$

with $y = x$. That is, the directional derivative of $f(x, y)$ in the *different* direction, y = constant, must vanish at a point on the line $y = x$, as occurs at B in Fig. 2.

Because the variational integral is not even stationary in a restricted variational principle, the exact value $\phi(0, 0)$ of the local potential is approximated only to the first degree in ϵ by a trial solution. Thus (compare equation 44)

$$\phi(\epsilon, \epsilon) = \phi(0, 0) + \delta_T \Phi + 0(\epsilon^2). \qquad (53)$$

In contrast a true variational principle provides approximation to the second degree in the magnitude factor ϵ, and this is an important advantage over a restricted principle, so far as computation of a variational integral of physical significance is concerned.

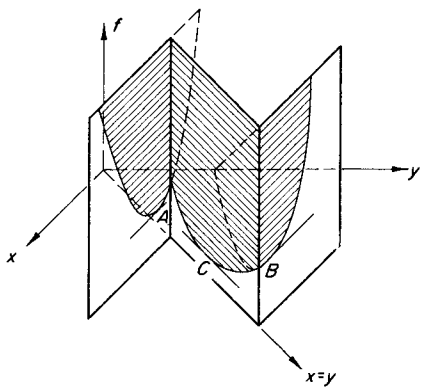

FIG. 2. Geometric interpretation of restricted variations. A: $\partial f(x, y)/\partial x = 0$; B: $[\partial f(x, y)/\partial x]_{x=y} = 0$, restricted variational principle; C: $df(x, x)/dx = 0$, variational principle.

In the so-called self-consistent approximation scheme based on the local potential the temperature is expanded in terms of a chosen set of functions of position and time containing N adjustable constants, α_i, which are evaluated to make $\delta_{T_0}\Phi = 0$.† Thus the trial solution is of the form

$$T^* = T^*(\mathbf{x}, t; \alpha_i). \qquad (54)$$

The alias temperature is represented by exactly the same functional form, but with an ostensibly different set of N constants:

$$T_0^* = T^*(\mathbf{x}, t; \beta_i). \qquad (55)$$

Substituted in equation (42) these forms make the local potential a function of the adjustable constants α_i and β_i. The approximate solution is found by solving the N equations

$$\left[\frac{\partial \Phi(\alpha_i, \beta_i)}{\partial \alpha_j}\right]_{\alpha_i = \beta_i} = 0 \qquad (56)$$

for the equally numerous constants, α_i. These equations are, in more explicit form

$$\int_\theta^t \int_v \frac{\partial T^*}{\partial \alpha_j}\left[\rho C_v^* \frac{\partial T^*}{\partial t} - \nabla \cdot (k^* \nabla T^*)\right] dV\, dt + \int_\theta^t \int_v \frac{\partial T^*}{\partial \alpha_j}\left[k^* \mathbf{n} \cdot \nabla T^* + h_s^*(T^* - T_s)\right] dS\, dt = 0 \qquad (57)$$

where T^* stands for a trial solution as in equation (54).†

Galerkin's method is applied to the same problem as follows. Temperature is approximated by the same form of trial solution, equation (54), which is substituted into the differential equation and boundary conditions, equations (34) and (35), to form what are called residuals. The residuals are required to be orthogonal, in the functional analysis sense, to each of the weighting functions; thus each is multiplied by the weighting function $\partial T^*/\partial \alpha_j$, integrated over the volume and surface, respectively, and added to give exactly equation (57). Consequently the approximate solution is

† The temperature can also be expanded in terms of a given set of functions of position containing undetermined functions of time; ordinary differential equations for the latter would emerge. To date, however, the local potential method seems not to have been applied in this, the fashion of Lagrangian thermodynamics (see below).

† Multiplying each of these equations by the corresponding $\delta\alpha_j$ and adding the products together regenerates equation (39), inasmuch as the variational of the trial solution, T^*, is by definition $\delta T^* = \sum(\partial T^*/\partial \alpha_j)\delta\alpha_j$.

precisely the same as that obtained by the local potential method, and without recourse to any variational formalism.

This is an important distinction. The Galerkin method proceeds directly from the original equations to obtaining the weighted residuals—the left-hand-side of equation (57). The local potential method requires intermediate steps of deriving or devising anew a local potential and then taking its variation. Galerkin's method is plainly more straightforward. The equivalence can be shown for *any* problem treated by the local potential method in the same fashion.

There is another important comparison, which concerns the combination of volume and boundary residuals. These have been added to get equation (57); whether they should be added or subtracted is decided in exactly the same way as was used to decide whether to add or subtract equation (37) and (38) to get equation (39) in the derivation of the local potential.† This means that natural boundary conditions can be accommodated by the Galerkin method with no more or less difficulty than they are by any variational formulation, including restricted variational principles of the sort under examination.

The local potential method has no advantage over the Galerkin method in regard to natural boundary conditions, and it is conceptually more involved. As has been shown, the local potential is not stationary with respect to temperature and therefore is unlikely to be as closely approximated as a stationary variational integral would be by means of a trial solution for temperature T and $T_0 = T$. Moreover, the approximate value of the local potential (if indeed its value is of any physical significance) may equally well be above or below the true value and it may increase or decrease with successive approximations. These points have been obscured by many claims that the local potential formulation is a minimum principle [22, 25, 19, 44]. However true that may be in the peculiar situation that the temperature alias T_0 is a definite, known function of position and time but T is not, it is obviously not true in the practical and real problem of solving equations (34–36) for the temperature field. In practice neither T_0 nor T would be known and both would have to be approximated.

The local potential formulation does lead to an iteration scheme for generating an approximate solution: the last approximation is adopted for T_0 and used to calculate T, its successor. So far this scheme has been applied to one-dimensional, nonlinear, steady state heat conduction [20, 49]. Even its advocates grant that the calculations rapidly increase in complexity with successive approximations. The convergence of the iteration has recently been examined [28]. Final evaluation of the iteration scheme will require its application to more difficult problems, particularly unsteady-state ones.

Any information indicating that an approximation method converges on the exact solution sought is likely to be reassuring to anyone attempting to determine stationary states or transient evolution of a system. Convergence of the Galerkin method has been treated for certain classes of linear boundary value and eigenvalue problems [33] and for nonlinear integral equations [27].† While Glansdorff [19] recently mentioned a convergence proof which is said to depend crucially on the local potential and to pertain to steady-state heat conduction in three-dimensions, the type of convergence and the details of the proof were left to a future publication. It seems likely that the chief source of information about the underlying mathematical aspects of the local potential method will be studies of the Galerkin method to which it is equivalent.

In favor of the local potential formalism it can be pointed out that the concept of the local potential was introduced in connection with

† Combination of volume and surface residuals has proved useful in treating various problems by Galerkin's method [14, 16].

† See also the review [16] for a listing of other proofs of convergence that are related.

what is called an evolution criterion [23, 22], in which context it may have theoretical utility unrelated to the practical matter of approximate solution to problems of predicting system performance. More recently the local potential has been interpreted in the light of fluctuation theory [36, 37], but this does not appear to alter the status of the local potential formulation as a restricted variational principle. While the local potential might be said to permit diverse irreversible phenomena to be summarized or even unified under one evolution criterion, it does suffer the anomaly that not one but rather several local potentials exist for almost any given problem.

Roberts [38] has shown that to the first order of approximation a local potential exists for any problem. In fact the local potential depends on the manner of introducing alias variables; this is strictly a matter of choice, and different choices produce different local potentials. For example, in simple steady-state heat conduction problems three possible local potentials are [15]

$$\Phi[T, T_0] \equiv \int_v k_0 T_0^2 [\nabla(1/T)]^2 \, dV \qquad (58)$$

$$\Phi[T, T_0] \equiv \int_v k_0 T_0 (\nabla \ln T)^2 \, dV \qquad (59)$$

$$\Phi[T, T_0] \equiv \int_v k_0 (\nabla T)^2 \, dV \qquad (60)$$

which correspond, respectively, to the rate of entropy production, the non-compensated heat of Clausius, and the familiar but unnamed integrand in Dirichlet's principle. In the first applications of the local potential (60) leads to computations which are *beaucoup plus simples* [20] than those to which (58) and (59) lead; the latter computations are equivalent to versions of the method of moments which are closely related but more cumbersome than the Galerkin method [15]. While Glansdorff *et al.* [20] kept (60) in the background because it did not occur explicitly in their evolution criterion, later users have bowed to practical expedience—Hays [25] and Schechter [44] employ local potentials analogous to (60) exclusively.

Finally, the local potential method has no demonstrated utility in formulating new constitutive relations for irreversible phenomena. It would appear to be more efficient and probably safer to relate flux or rate to configurational variables in the usual way than to postulate new forms of local potential. To date, at least, the benchmarks in published discussions of the method have been familiar differential equations; once these and the boundary conditions are in hand there is no practical need for a local potential although one or more can be derived for the problem of interest.

4. INEXACT VARIATIONS

By making use of infinitesimal functions of time, a kind of inexact variation, Biot [3, 4, 5] and others have forced the analysis of heat transport and related processes into a mold patterned roughly after variational formalism employed in mechanics and represented by equations (4) and (18) above. Biot's treatment, named Lagrangian Thermodynamics, centers on a "variational principle" which is in fact a quasi-variational formulation, i.e. the quantity required to vanish is neither the variation of a functional nor even the instantaneous variation of a function. The stated purpose of the "variational principle" is to permit approximate solution of problems involving nonlinear property variations and boundary conditions. The approximation method that emerges from Lagrangian Thermodynamics is equivalent to Galerkin's method, as the authors have shown in an earlier paper [14]. The equivalence was there illustrated by the case of heat conduction; here convective transport will be considered right along with conduction in order to study in greater depth the consequences of that equivalence.

The basic equations when the flow is incompressible and when Fourier's law is satisfactory are

$$\rho C_v \frac{\partial T}{\partial t} + \rho C_v \mathbf{u} \cdot \nabla T - \nabla \cdot (k \nabla T) = 0 \quad \text{in } V, \quad t > 0 \qquad (61)$$

$$k\mathbf{n}\,.\,\nabla T + h_s(T - T_s) = 0$$

$$\text{on} \quad S, \qquad t > 0 \tag{62}$$

$$T = \psi(x) \qquad \text{in} \quad V, \qquad t \leqslant 0. \tag{63}$$

The heat-transfer coefficient is denoted h_s and is a known function of position and time on the boundary, as is the external temperature field T_s also. Biot defines the "total heat", a quantity dependent on the choice of temperature datum:

$$h \equiv \int_0^T \rho C_v \, \mathrm{d}T, \tag{64}$$

and he introduces a "heat-flow vector" field, $\mathbf{H}$, so defined that

$$h = -\nabla\,.\,\mathbf{H} \quad \text{in} \quad V \tag{65}$$

$$\mathbf{n}\,.\,\frac{\partial \mathbf{H}}{\partial t} = k\mathbf{n}\,.\,\nabla T \quad \text{on} \quad S. \tag{66}$$

That is,

$$\mathbf{H} = +\frac{1}{4\pi}\nabla\left[\int \frac{h(x')}{|\mathbf{x}' - \mathbf{x}|}\mathrm{d}V'\right] + \nabla \times \mathbf{A} \tag{67}$$

where $\mathbf{A}$ is an arbitrary vector field: $\mathbf{H}$ is not uniquely defined. Defining the "thermal potential", a function of time,

$$V \equiv \int_v \int_0^h T \, \mathrm{d}h \, \mathrm{d}V \tag{68}$$

so that

$$\delta_t V = \int_v T \delta_t h \mathrm{d}V = -\int T \nabla\,.\,\delta_t \mathbf{H} \mathrm{d}V. \tag{69}$$

Biot goes on to set up two inexact variations† under the name "variational invariants":

$$\left.\begin{aligned} \widehat{\delta D} &\equiv \int_v \frac{1}{k}\left(\frac{\partial \mathbf{H}}{\partial t} - h\mathbf{u}\right)\,.\,\delta_t \mathbf{H}\,\mathrm{d}V, \\ \widehat{\delta D}_s &\equiv \int_S \frac{1}{h_s}\,\mathbf{n}\,.\left(\frac{\partial \mathbf{H}}{\partial t}\right)\mathbf{n}\,.\,\delta_t \mathbf{H}\,\mathrm{d}S. \end{aligned}\right\} \tag{70}$$

His "variational principle" relies on these; it is expressed as a variational invariant

$$\delta_t V + \widehat{\delta D} + \widehat{\delta D}_s = -\int_S T_s \mathbf{n}\,.\,\delta_t \mathbf{H}\,\mathrm{d}S \tag{71}$$

where $\delta_t \mathbf{H}$ is an instantaneous variation [see footnote to equation (37)]. This is a quasi-variational statement, for all four terms are functions of time and of them only one is generally the instantaneous variation of an integral over the system. By manipulating equation (69) it is possible to rearrange equation (71) to give

$$\int_v \delta_t \mathbf{H}\,.\left[\nabla T + \frac{1}{k}\left(\frac{\partial \mathbf{H}}{\partial t} - h\mathbf{u}\right)\right]\mathrm{d}V + \int_S \mathbf{n}\,.\,\delta_t \mathbf{H}\left[T_s - T + \frac{1}{h_s}\mathbf{n}\,.\,\frac{\partial \mathbf{H}}{\partial t}\right]\mathrm{d}S = 0. \tag{72}$$

Formally, the "Euler equation" and "natural boundary condition" are

$$\nabla T + \frac{1}{k}\left(\frac{\partial \mathbf{H}}{\partial t} - h\mathbf{u}\right) = 0 \quad \text{in} \quad V \tag{73}$$

$$(T_s - T) + \frac{1}{h_s}\mathbf{n}\,.\,\frac{\partial \mathbf{H}}{\partial t} = 0 \quad \text{on} \quad S. \tag{74}$$

The divergence of k times equation (73) gives (61), while (74) with (66) gives (62); thus the quasi-variational formulation does reproduce the original differential equation system.

In the variational method based on this formulation, the auxiliary field $\mathbf{H}$ is approximated by a chosen functional form containing a finite number of parameters that are unknown functions of time:

$$\mathbf{H}^* = \mathbf{H}^*[\mathbf{x}, t; q_i(t)]. \tag{75}$$

The functions $q_i(t)$, which are analogous to the variational parameters in the classical variational method, are named "generalized coordinates" by Biot, who unfortunately failed to distinguish between exact and trial solutions. A convenient form for the trial solution is a linear expansion in terms of a suitable set of functions of position (also employed by Rosen—see above):

$$\mathbf{H}^* = \sum_{i=1}^{N} q_i(t)\,\mathbf{f}_i(\mathbf{x}). \tag{76}$$

† As in equation (1) above, the overbars in (70) denote infinitesimals which cannot be expressed as variations of other quantities.

In any case, with the definition $\mathbf{H}_i^* \equiv \partial \mathbf{H}^*/\partial q_i$, which is used by Biot, the variation in $\mathbf{H}^*$ resulting from instantaneous variation of the values of $q_i(t)$ can be written $\delta_t \mathbf{H}^* = \sum \mathbf{H}_i^* \, \delta q_i$. Accordingly, when the trial solution $\mathbf{H}^*$, the corresponding h^* from equation (65), and the solution of equation (64) for T^* are all substituted in the "variational principle", equation (72), and the q_i are recognized as independent of one another, the variational method emerges as

$$\int_V \frac{\partial \mathbf{H}^*}{\partial q_i} \cdot \left[\nabla T^* + \frac{1}{k^*} \left(\frac{\partial \mathbf{H}^*}{\partial t} - h^* \mathbf{u} \right) \right] \mathrm{d}V + \int_S \mathbf{n} \cdot \frac{\partial \mathbf{H}^*}{\partial q_i} \left[T_s - T^* + \frac{1}{h_s^*} \mathbf{n} \cdot \frac{\partial \mathbf{H}^*}{\partial t} \right] \mathrm{d}S = 0. \tag{77}$$

This is a set of N ordinary, first-order differential equations for the N functions $q_i(t)$. Initial conditions must be deduced from equation (63).

To apply the Galerkin method to equations (73) and (74) one substitutes a trial solution (75) into the equations to form the local residuals, integrates them with weighting functions $\mathbf{H}_i^*$ and $\mathbf{n} \cdot \mathbf{H}_i^*$, respectively, adds the weighted residuals and puts the sum equal to zero. The result is just equation (77). Hence the approximate solution is the same as that obtained by Biot's method, and requires no intermediate steps of variational formalism.

Nearly all published applications of Biot's method (see Lardner's review [30] have been to one-dimensional problems, for which the auxiliary field $\mathbf{H}$ is a parallel vector field easily obtained by quadrature. However, for two- and three-dimensional problems the computations become unwieldly [4] and Biot's method of approximation loses whatever attractiveness of simplicity it may hold for one-dimensional transport. The difficulty is that one is supposed to satisfy equation (65) and (66) exactly and it is usually easier to assume a trial solution for the temperature field, T^*, from which the "total heat" field, h^*, follows by integration, than it is to choose a "heat-flow vector" field, $\mathbf{H}^*$. Accordingly $\mathbf{H}^*$ must be gotten from h^* by means of equation (67); i.e. by solving a partial differential equation. The equivalent Galerkin scheme, using $\mathbf{H}^*$, suffers this same deficiency, but of course the Galerkin method can and probably should be applied directly to the original transport problem, equations (61–63), without introducing the artifice, $\mathbf{H}$. The latter plays no essential role and is certainly unnecessary for splitting equation (61) back down into the equation of change and Fourier's law in order to control the distribution of residual between these two parts of the problem [14].

From the standpoint of approximate solutions Lagrangian Thermodynamics offers no advantages not already available from MWR. The question of its theoretical significance remains. Biot's papers [3, 4, 5] convey the impression that his variational formulation is somehow linked with irreversible thermodynamics and a "general principle of minimum entropy production". In particular, these papers imply that there exist functionals or functions $D(\mathbf{H})$ and $D_s(\mathbf{H})$, the variations of which are the infinitesimals δD and δD_s in equation (71); Biot refers to these hypothetical quantities as volume and surface "dissipation functions". There is also the matter of the choice of name, "Lagrangian Thermodynamics".

In strict logic, Biot's constructions pertain not to the quasi-variational principle, equation (71), but to the commonplace set of equations (77) for the finite number, N, of functions $q_i(t)$ in a particular choice of trial solution, $\mathbf{H}^*$. Because

$$\left(\frac{\partial \mathbf{H}^*}{\partial t} \right)_x = \left(\frac{\partial \mathbf{H}^*}{\partial t} \right)_{x, q_i} + \sum_{i=1}^{N} \left(\frac{\partial \mathbf{H}^*}{\partial q_i} \right) \dot{q}_i \tag{78}$$

$$\frac{\partial}{\partial \dot{q}_i} \left(\frac{\partial \mathbf{H}^*}{\partial t} \right) = \frac{\partial \mathbf{H}^*}{\partial q_i} \tag{79}$$

it follows that (77) can be written in the form of the Lagrangian equations for an inertialess, mechanical system of discrete elements with

viscous damping and nonconservative as well as conservative forces [24]:†

$$\frac{\partial V^*}{\partial q_i} + \frac{\partial (D^* + D_s^*)}{\partial \dot{q}_i} = Q_i^* \tag{80}$$

provided the following definitions are made:

$$\left.\begin{aligned} V^* &\equiv \int_v \int_\theta^h T^* \, \mathrm{d}h^* \, \mathrm{d}V, \\ D^* &\equiv \frac{1}{2} \int_v \frac{1}{k^*} \left(\frac{\partial \mathbf{H}^*}{\partial t} - h^* \mathbf{u} \right)^2 \mathrm{d}V \\ Q_i^* &\equiv - \int_S T_s \mathbf{n} \cdot \mathbf{H}_i^* \, \mathrm{d}S, \\ D_s^* &\equiv \frac{1}{2} \int_v \frac{1}{h_s^*} \left(\mathbf{n} \cdot \frac{\partial \mathbf{H}^*}{\partial t} \right)^2 \mathrm{d}V. \end{aligned}\right\} \tag{81}$$

These are all functions of time which depend on the functions $q_i(t)$ in the particular choice of $\mathbf{H}^*$. If V^* is regarded as independent of the functional form of $\mathbf{H}^*$ one can write its variation as

$$\delta V^* = \sum \frac{\partial V^*}{\partial q_i} \delta q_i. \tag{82}$$

Only by adopting Biot's singular definition of the variation of a "dissipation function" with respect to "generalized coordinates" can one write

$$\delta_B D^* \equiv \sum \frac{\partial D^*}{\partial \dot{q}_i} \delta q_i, \qquad \delta_B D_s^* \equiv \sum \frac{\partial D_s^*}{\partial \dot{q}_i} \delta q_i. \tag{83}$$

Then one can put the set of equations (77) in yet another notational dress,

$$\delta V^* + \delta_B (D^* + D_s^*) = \sum Q_i^* \, \delta q_i \tag{84}$$

which bears a purely superficial resemblance to the quasi-variational principle, equation (71). Biot evidently identified (71) and (84), using the same notation and indeed the same equation to stand for both, however. It is now clear that $\delta \widehat{D} + \delta \widehat{D}_s$ in the former refers to the exact solution $\mathbf{H}$ while $\delta_B(D^* + D_s^*)$ in the latter refers to a particular form of approximate solution, $\mathbf{H}^*$, in which only the functions $q_i(t)$ can be varied. The possibility of defining D^* and D_s^* in no way implies the existence of quantities $D(\mathbf{H})$ and $D_s(\mathbf{H})$.

On the basis of equation (73), which is satisfied only by an exact solution $\mathbf{H}$, Biot asserted in effect that

$$\frac{\partial \mathbf{H}^*}{\partial t} - h^* \mathbf{u} = - k^* \Delta T^* \tag{85}$$

and that

$$D^* = \tfrac{1}{2} \int_v k^* (\nabla T^*)^2 \, \mathrm{d}V \tag{86}$$

neither of which is in general true. The latter expression resembles but is not identical with the rate of entropy generation by heat conduction [compare equations (22) and (58)] and this irrelevant resemblance was cited [5] as the link with irreversible thermodynamics. Finally, Biot referred to an earlier hypothesis [2], to which the foregoing criticisms also apply:†

> Considering a system which is not in equilibrium, its instantaneous velocity direction is such that the rate of entropy production is a minimum for all possible velocity vectors satisfying the condition that the power input of the disequilibrium forces is constant.

In the context of heat transfer in flow systems this questionable statement evidently is held to mean that

$$\delta_{q_i} (D^* + D_s^*) \equiv \frac{\partial (D^* + D_s^*)}{\partial \dot{q}_i} \delta \dot{q}_i = 0 \tag{87}$$

with the constrain that

$$\sum \left(Q_i^* - \frac{\partial V^*}{\partial q_i} \right) \dot{q}_i = 0 \tag{88}$$

† The Lagrangian equations for such a system cannot be derived as the Euler equations of a true variational principle, it should be noted.

† To begin with, there is a tacit assumption that a *continuous* system can be completely described in terms of a *finite* number of "generalized coordinates". This assumption is paralleled in [5] by the lack of distinction between $\mathbf{H}[x, t]$ and $\mathbf{H}^*[\mathbf{x}, t; q_i(t)]$.

where yet another special type of variation must be employed—this time variation with respect to the $\dot{q}_i$ with the q_i themselves, somehow held fixed, as in Chambers's scheme [7], mentioned above. Formally, with a Lagrangian multiplier set equal to unity, this does reproduce equation (80) and thus equation (77) for the functions q_i in a trial solution. This is no true minimum principle; at the most (87) and (88) amount to a restricted variational formulation for the q_i, which is scarcely a principle more general than those of the thermodynamics of irreversible processes, as has been claimed [5]. Furthermore, this "principle" applies only to the approximate solution involving H^* and $q_i(t)$, not the exact solution having no $q_i(t)$.

From the standpoints of physical theory and mathematical analysis it appears that the only significance that can be attached to Biot's quasi-variational formulation and notation in the style of Lagrangian equations is as a disguise for Galerkin's method of determining unknown functions in a trial solution.

5. CONCLUSIONS

The quasi-variational formulations and restricted variational principles that have appeared in the literature depart to such an extent from the classical calculus of variations that, as summarized in Table 1, they do not possess the advantages associated with genuine variational principles. Behind the formulations of Rosen, Glansdorff and Prigogine, Biot, and others lies the notion of a general minimum principle related to the so-called principle of minimum entropy production for irreversible processes. No such principle has ever been established, however, except for certain isothermal approximations to the behavior of quite special systems. Onsager's "variation principle", so often adverted to, reproduces a constitutive equation relating flux to field configuration (e.g. temperature) when the latter is known; it cannot stand in for the basic equation of change of that configuration. From a mathematical point of view it appears that no *general* variational principle can be devised for transport and transformation processes, despite the alluring hope expressed by the mathematician Euler in 1744 and not forgotten since:

> As the construction of the universe is the most perfect possible, being the handiwork of an all-wise Maker, nothing can be met with in the world in which some maximal or minimal property is not displayed. There is, consequently, no doubt but that all the effects of the world can be derived by the method of maxima and minima from their final causes as well as from their efficient ones.

Having long since added stationary quantities to the hoped-for maximal and minimal ones, the searchers have had to distort and depose the definitions from the calculus of variations in order to make progress. The writers hold the view that variational formulations arrived at in this way are unjustifiably called principles and are all too frequently misinterpreted or misrepresented and, on the other side, misunderstood.

The formulations examined here all rest directly on basic equations of change and familiar constitutive relations and boundary conditions. They possess no power in synthesizing descriptions of new types of systems and materials. Constitutive equations and boundary conditions are better postulated as such than as forms of functions in some integral or infinitesimal functional.

What practical utility the variational formulations have results from the corresponding variational methods for approximate solutions of problems of predicting performance of physical systems. But in fact these approximation schemes are far more readily set up as the straightforward Galerkin method or another closely related version of the method of weighted residuals. That these direct approximation procedures avoid completely the effort and mathematical embellishment of a variational formulation has not been emphasized adequately in the literature. Yet the significance of the

variational formulations is clarified by viewing them in the light of MWR. The interrelationships and equivalences of many of these approximation methods are summarized in Fig. 2. Apart from self-adjoint, linear systems, which are comparatively rare, there is no practical need for variational formalism. When approximate solutions are in order the applied scientist and engineer are better advised to turn immediately to direct approximation methods for their problems, rather than search for or try to understand quasi-variational formulations and restricted variational principles.

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Résumé—On examine plusieurs tentatives de formulation de principes variationnels pour des systèmes non auto-adjoints et non-linéaires. On trouve que les formulations variationnelles ne possèdent pas les avantages des principes variationnels véritables, principalement parce que l'intégrale variationnelle n'est pas stationnaire ou parce qu'il n'existe pas d'intégrale variationnelle. Les méthodes d'approximations variationnelles correspondantes sont équivalentes à la méthode plus directe de Galerkin ou à une autre version de la méthode des résidus pondérés qui lui est reliée étroitement. Les méthodes dues à Rosen (variations restreintes), à Glansdorff et Prigogine (potentiel local) et à Biot (thermodynamique lagrangienne) sont traitées. On en conclut que l'on n'a pas besoin pratiquement de formulations variationnelles de l'espèce étudiée.

Zusammenfassung—Verschiedene Versuche, Variationsprinzipien für nicht selbst adjungierte und nichtlineare Systeme zu formulieren wurden überprüft. Die Variationsformulierungen zeigen einen Mangel an echten Variationsprinzipien, vor allem deshalb weil das Variationsintegral nicht stationär ist oder nicht existiert. Für die entsprechenden Näherungsvariationsmethoden wird gezeigt, dass sie äquivalent der etwas direkteren Galerkin-Methode sind oder einer anderen eng verwandten Version der Methode der gewogenen Residuen entsprechen. Die Methoden nach Rosen (beschränkte Variationen), Glansdorf und Prigogine (örtliches Potential) und Biot (Lagrangsche Thermodynamik) werden behandelt. Als Schlussfolgerung wird keine praktische Notwendigkeit für die hier untersuchten Variationsformulierungen erkannt.

Аннотация—Сделана попытка сформулировать вариационные принципы несамосопряженных и нелинейных систем. Найдено, что у вариационных формулировок нет преимуществ истинных вариационных принципов, в основном из-за того, что вариационный интеграл не является стационарным или из-за того, что не существует никакого вариационного интеграла. Показано, что существующие вариационные методы аппроксимации эквивалентны более прямому методу Галеркина или другому близко связанному

с ним варианту метода взвешенных разностей. Рассмотрены методы Розена (ограниченные вариации), Гландсдорфа и Пригожина (локальный потенциал) и Био (термодинамика в лагранжевой формулировке). Сделан вывод, что в вариационых формулировках рассмотренного типа нет практической необходимости.