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ADJOINT VARIATIONAL PRINCIPLES FOR CONVECTIVE DIFFUSION

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Abstract—Following a suggestion due to Morse and Feshbach, adjoint variational principles are constructed for unsteady convective diffusion of a passive scalar, such as heat or mass, in an incompressible fluid under conditions of considerable generality. By recourse to the classical theory of fields, sufficiency conditions are established for an extremal principle. A simple illustrative example is adduced.

I. INTRODUCTION

SINCE Onsager's [10] introduction of a dissipation function, taken to be one-half the rate of irreversible production of entropy, as an invariant in dissipative processes, the problem of a variational principle for the heat equation, in its various forms, has occupied the attention of a number of investigators. Rosen [11] and Chambers [3] were able to derive suitable Lagrange densities, valid, however, under highly restrictive conditions. It remained for Biot [1] to present a formalism exactly analogous to that of mechanical dissipative systems, so that quite general problems in the conduction of heat in anisotropic solids could be solved. Biot and Daughaday [2] later extended the application of the formalism to the ablation of slabs and Nigam and Agrawal [9] and Gupta [6] to convective heat transfer in an incompressible fluid.

In this note we elaborate upon a suggestion by Morse and Feshbach [8] for the construction of an adjoint variational principle, which does not seem to have been pursued in the engineering literature. The basic idea is the following: consider a second-order dissipative operator, L, defined on some space-domain, V for time $t \geqslant 0$, subject to certain boundary conditions on the surface, S, of V, and initial conditions at $t = 0$, Then, form the functional

$$J = \int_0^t \int_V \varphi^* L\varphi \, dv \, d\tau \tag{1}$$

where φ and φ^* will henceforth be termed the original and adjoint variables, respectively. Its first variation, assuming the surface to be fixed, is given by

$$\delta J_1 = \int_0^t \int_V [\delta\varphi^* L\varphi + \varphi^* L\delta\varphi] \, dv \, d\tau \tag{2}$$

assuming the commutativity of L and the variation operator. Now, by integrating by parts and by use of Green's theorem, the second term can be written

$$\int_0^t \int_V \varphi^* L\delta\varphi \, dv \, d\tau = -\int_0^t \int_V \delta\varphi \tilde{L}\varphi^* \, dv \, d\tau + \int_0^t P_1|_S \, d\tau + \int_V P_2|_{\tau=0}^{\tau=t} \, dv \tag{3}$$

where $\tilde{L}$ is the adjoint operator, and P_1 and P_2 are functions of φ^*, $\delta\varphi$, and their derivatives with respect to space and time. Then the vanishing of the first variation requires that

$$L\varphi = 0 \tag{4}$$

$$\tilde{L}\varphi^* = 0 \tag{5}$$

in the domain V for $t \geqslant 0$. In addition, if the boundary conditions for φ are prescribed at S and at $t = 0$, appropriate boundary and "initial" conditions on φ^* are those which make the last two integrals in equation (3) vanish. Equations (4) and (5) are the Euler–Lagrange equations for the variational principle $\delta J = 0$. If the kernel of equation (1) is designated by $K_1 = \varphi^* L\varphi$, it is evident that $K_2 = \varphi\tilde{L}\varphi^*$, or any linear combination of K_1 and K_2, leads to the

same Euler–Lagrange equations.† Further, one can form $K(\varphi^*, \varphi)$, a homogeneous quadratic function of φ, φ^*, and their first derivatives in space and time (called the Lagrange density), by application of Green's theorem and integration by parts. It can be seen that the Lagrange density, and hence the variational principle, is not unique, although all principles having the same Euler–Lagrange equations can be transformed into one another by addition of suitable surface integrals.

The subject has now been brought into the framework of the classical theory of fields, from which many of the results can be directly applied. In particular, a Hamiltonian density, which has the dimensions of an energy density, can be identified, whose integral over the volume V, under suitable restrictions, remains constant with time. In this event, the adjoint system represents a "mirror-image" system into which the energy dissipated in the physical system drains. The equations of motion can be written in Hamilton's canonical form, although, as a consequence of the fact that the Lagrange density is linear and not quadratic, this does not result in a transformation to a new set of state variables. As a consequence, Hamilton's equations lead right back to the original equations of motion. Energy flux density vectors for the extended system can also be identified. An interesting subject for future investigation, which is not further considered here, is the possible application of the Hamilton–Jacobi theory, with its well-known connection to the theory of geometric optics, to the extended system.

II. STATEMENT OF THE PROBLEM

To make matters more concrete, consider the general problem of unsteady convective diffusion of heat in an incompressible fluid of specified velocity. For the present, the fluid properties are assumed to be temperature-independent, although they may be specified functions of position. The removal of this restriction will be discussed later. The volume occupied by the fluid may be finite or infinite in extent, simply or multiply connected, open or closed. The last distinction determines whether fluid enters the volume from outside points.

The governing differential equation is then

$$T,_4 + U_j T,_j - (\alpha T,_j),_j - Q = 0 \qquad (6)$$

where the Cartesian space-time variables‡ are given by $\xi_m = x, y, z, t; m = 1, 2, 3, 4$. Commas denote partial differentiation, and the Einstein summation convention is used throughout, the subscripts m and n to be summed over 1, 2, 3, 4, and j over 1, 2, 3. T,α and U_j represent the temperature, thermal diffusivity, and velocity components of the fluid at any point. Q, the instantaneous strength of the distributed heat source, which includes the viscous dissipation term, is at present assumed to be of the form $Q = f_1(\xi_m)T + f_2(\xi_m)$, where f_1 and f_2 are specified functions of position and time.

The initial condition is

$$T = T_0(\xi_j) \quad \text{at} \quad \xi_4 = 0 \qquad (7)$$

On the surface S a very general boundary condition is imposed:

$$T,_j\gamma_j + \beta T = g \quad \text{on } S_1 \text{ for } 0 < \xi_4 \leqslant t \qquad (8)$$

where γ_j are the direction cosines of the outward normal to the surface, and β and g are prescribed (not necessarily continuous) functions of the surface co-ordinates and time. This non-homogeneous boundary condition of the third kind is the most general linear boundary condition involving only the temperature and its normal gradient. Homogeneous boundary conditions, and boundary conditions of the first and second kind (specified surface temperature and heat flux) can be obtained as special cases by a

† In particular, the adjoint operator is usually defined by the equivalence of the volume integral of the kernel $(K_1 - K_2)$ to a surface integral. This is the basis of the approach employed by Goodman [12] in solving for an unknown surface temperature or heat flux in heat conduction problems by a non-variational technique.

‡ Cartesian tensors are used to avoid obscuring the essential details. No difficulty is experienced in transforming to more general metrics, Also, the notation treats space and time variables on an equal footing. This has some advantages later in treating the stress-energy tensor. In this four-dimensional space the application of Green's theorem over a domain R, where the point $P(\xi_m) \in R$, is equivalent to the use of Green's theorem over the three-volume, V, together with integration by parts with respect to time.

limiting process involving β and g over portions of the surface.

The adjoint system for the space-time domain satisfies the time-reversed equation

$$T^*_{,4} + U_j T^*_{,j} + (\alpha T_{,j})_{,j} + f_1 T^* + f_2 = 0 \quad (9)$$

The adjoint "initial" condition is time-reversed:

$$T^* = T_0(\xi_j) \quad \text{at} \quad \xi_4 = t \quad (10)$$

while the adjoint boundary condition is taken to be

$$T^*_{,j}\gamma_j + \left(\beta + \frac{1}{\alpha} U_j\gamma_j\right) T^* = g \quad \begin{matrix}\text{on } S \\ 0 \leqslant \xi_4 < t\end{matrix} \quad (11)$$

The reason for this choice will shortly become clear. Note that the original and adjoint boundary conditions are identical only if no fluid passes through S. Finally, the incompressibility stipulation requires that

$$U_{j,j} = 0 \quad (12)$$

Other restrictions, in the form of admissibility conditions, will appear in the discussion.

III. CONSTRUCTION OF A VARIATIONAL PRINCIPLE

We begin by seeking a Lagrange density whose Euler–Lagrange equations are the governing differential equations (6) and (9). Such a density is

$$L = \alpha T_{,j} T^*_{,j} + \tfrac{1}{2}(T^* T_{,4} - T T^*_{,4}) + \tfrac{1}{2} U_j (T_{,j} T^* - T^*_{,j} T) - T f_1 T^* - f_2 (T + T^*) \quad (13)$$

satisfying the Euler–Lagrange equations

$$\frac{\partial L}{\partial T} = \left(\frac{\partial L}{\partial T_{,m}}\right)_{,m}; \quad \frac{\partial L}{\partial T^*} = \left(\frac{\partial L}{\partial T^*_{,m}}\right)_{,m} \quad (14)$$

By substitution of equation (13) into equation (14), it is readily verified that these are equivalent to equation (6) and equation (9). Equation (14) arises from the variational principle $\delta J = 0$, where

$$J = \int_0^t \int_V L \, dv \, d\xi_4 \quad (15)$$

and $dv = d\xi_1 \, d\xi_2 \, d\xi_3$. This may be written more compactly

$$J = \int_R L \, d\xi_m \quad (16)$$

where $d\xi_m = d\xi_1 \, d\xi_2 \, d\xi_3 \, d\xi_4$ and R: $\xi_j \in V$, $0 \leqslant \xi_4 \leqslant t$.

We turn now to the problem of satisfying the initial and boundary conditions. One obvious approach is to limit trial functions to those which satisfy these conditions. For simple cases this will be a preferred procedure, but for more complicated problems it is difficult to construct admissible trial functions. It is then preferable to make these conditions appear as Euler–Lagrange equations by suitable modification of the principle. Thus, by adding surface integrals to J, one obtains

$$J' = J + \int_0^t \int_S \alpha[\beta_1 T T^* - (T + T^*)g] \, ds \, d\xi_4 + \int_V \tfrac{1}{2} T_0 (T^* - T) \Big|_{\xi_4 = 0}^{\xi_4 = t} dv \quad (17)$$

where β_1 is a function of space and time to be determined. On setting $\delta J' = 0$, one obtains on the four-surface, making use of equation (12):

$$\int_0^t \int_S [(\alpha T_{,j} - \tfrac{1}{2} U_j T)\,\delta T^* + (\alpha T^*_{,j} + \tfrac{1}{2} U_j T^*)\delta T]\gamma_j \, ds \, d\xi_4 + \int_V \tfrac{1}{2}(T^* \delta T - T \delta T^*) \Big|_{\xi_4 = 0}^{\xi_4 = t} dv + \alpha \int_0^t \int_S [(\beta_1 T - g)\delta T^* + (\beta_1 T^* - g)\delta T] \, ds \, d\xi_4 + \int_V \tfrac{1}{2} T_0 (\delta T^* - \delta T) \Big|_{\xi_4 = 0}^{\xi_4 = t} dv \quad (18)$$

where the first two integrals arise from the application of the four-space divergence theorem to the four-volume integral in equation (15). Upon collecting terms, the natural boundary conditions are seen to be

$$\begin{aligned} &T_{,j}\gamma_j - \frac{1}{2\alpha} U_j \gamma_j T + \beta_1 T = g \quad \text{on } S, \\ &\quad 0 < \xi_4 \leqslant t \\ &T^*_{,j}\gamma_j + \frac{1}{2\alpha} U_j \gamma_j T^* + \beta_1 T^* = g \quad \text{on } S \\ &\quad 0 \leqslant \xi_4 < t \end{aligned} \quad (19)$$

with the choice

$$\beta_1 = \beta + \frac{1}{2\alpha} U_j \gamma_j;$$

these equations reduce to the desired boundary conditions (8) and (11). However, in order to make the time-integrated terms in equation (18) vanish, it is necessary to restrict admissible trial functions to those which satisfy equations (7) and (10).

An alternative formulation of the variational principle is obtained with the aid of the four-space divergence theorem. The last term in equation (17) can be replaced by a volume integral $\int_R \frac{1}{2} T_0(T^* - T),_4 \, d\xi_m$. However, the integral over S in equation (17) presents difficulties, since it is not in suitable form for application of the divergence theorem. Re-writing it as

$$I = \int_0^t \int_S F_j \gamma_j \, ds \, d\xi_4, \text{ where } F_j = \alpha \gamma_j [\beta_1 TT^* - (T + T^*)g]$$

it can now be transformed into $\int_R F_{j,j} \, d\xi_m$, so that

$$J' = \int_R [L + F_{j,j} + \tfrac{1}{2} T_0(T^* - T),_4] \, d\xi_m \quad (20)$$

The two formulations are strictly equivalent, and since there may be difficulty in formulating a suitable vector function F_j which assumes the required values on S and whose divergence exists throughout V, there seems to be no particular advantage of equation (20). However, the method makes clear the construction of alternative variational principles. Thus, adding the four-divergence of the four-vector $(0, 0, 0, -\frac{1}{2} TT^*)$ to L, one obtains in place of equation (17).

$$J_1 = \int_R [L - \tfrac{1}{2}(TT^* + (T - T^*)T_0),_4] \, d\xi_m + I \quad (21)$$

On taking the variation, the time-integrated terms in equation (18) are now replaced by $-\int_V (T - T_0)\delta T^* \, |_{\xi_4 = 0}^{\xi_4 = t} \, dv$, which vanishes if trial functions for T^* only are restricted by admissibility initial conditions. The initial condition, equation (7), now appears as an Euler–Lagrange equation, so that the class of admissible functions has been enlarged.

IV. CLASSICAL THEORY OF FIELDS

The variational principle can be brought into a broader framework by relating it to the classical theory of fields [5], formulated by Hamilton, Jacobi, and others. The equivalence of a stationary property of the functional [equation (16)] with respect to arbitrary weak variations of the generalized co-ordinates, T and T^*, to the Lagrangian equations [equation (14)], is known as Hamilton's Principle, first formulated for dynamical systems. From the Lagrange density, L, one can construct the components of the "stress–energy" tensor, given by

$$W_{mn} = T,_m \frac{\partial L}{\partial T,_n} + T^*,_m \frac{\partial L}{\partial T^*,_n} - L\delta_{mn}$$

$$m,n = 1, 2, 3, 4 \quad (22)$$

If, in addition to the previous restriction of the physical properties being dependent only upon position, the flow is now taken to be steady, although not necessarily uniform, one can readily show that

$$W_{4j,j} + W_{44,4} = 0 \quad (23)$$

where W_{4j} are the components of the "energy-flow" vector, and $W_{44} = H$ is known as the Hamiltonian density. The proof is straightforward, since from equation (22)

$$W_{mn,n} = T,_{m,n} \frac{\partial L}{\partial T,_n} + T,_m \left(\frac{\partial L}{\partial T,_n}\right),_n - \left[\frac{\partial L}{\partial T} T,_m + \frac{\partial L}{\partial T,_n} T,_{n,m} + L,_j \delta_{mj}\right] \quad (24)$$

plus corresponding terms in T^*, since L is not an explicit function of time. Upon making use of equation (14), this reduces to

$$W_{mn,n} = -L,_j \delta_{mj} \quad (25)$$

which vanishes for $m = 4$, proving equation (23). For $m = 1, 2, 3$, $L,_j$ vanishes if the physical properties are constant, in view of equation (12).

The practical significance of all this lies in the fact that from equation (23)

$$\int_V W_{4j,j}\,dv = -\int_V W_{44,4}\,dv = -\frac{\partial}{\partial t}\int_V W_{44}\,dv = \int_S W_{4j\gamma j}\,ds \qquad (26)$$

upon applying Green's theorem. Now if the Hamiltonian energy density over the volume V is to remain constant with time, the surface integral on the right of equation (26) must vanish. This implies that the energy dissipated from the real system is drained into the adjoint system, so that the principle is a conservative one. This has computational advantages in that the stationary property for a conservative system corresponds to an extremal principle,† which assures convergence (although not necessarily to the correct answer). The convergence of the minimal sequence to the exact solution can be rigorously demonstrated for specialized conditions, such as the general linear elliptic partial differential equation with linear boundary conditions (7). In particular, the principle is a conservative one if the volume, V, extends over all space, and if the disturbance represented by the initial conditions vanishes at infinity. For a finite volume one can construct restricted conservative variational principles. Thus, employing the basic variational principle, equation (15),

$$W_{4j\gamma j} = T_{,4\gamma j}(\alpha T^*_{,j} + \tfrac{1}{2}U_j T^*) + T^*_{,4\gamma j}(\alpha T_{,j} - \tfrac{1}{2}U_j T) \qquad (27)$$

This vanishes everywhere on the surface S, if (1) the temperature and its adjoint are time-independent over the surface S, or (2) over positions of the surface where the real and adjoint temperatures are allowed to vary with time, the normal velocity and heat flux are both zero (corresponding to an adiabatic streamline or solid surface). In this event the integral of the Hamiltonian energy density over the volume V is independent of time. If a suitable vector function F_j can be found, a variational principle corresponding to equation (20) is applicable. $W_{4j\gamma j}$ then vanishes upon application of equations (8) and (11).

Finally, one can derive "canonical momentum densities" from equation (13):

$$P = \frac{\partial L}{\partial T_{,4}} = \tfrac{1}{2}T^*;\quad P^* = \frac{\partial L}{\partial T^*_{,4}} = -\tfrac{1}{2}T \qquad (28)$$

The adjoint temperature is thus proportional to the "momentum density", which bears little relationship to the momentum density of simple dynamical systems. As noted previously, the Lagrange density is linear, rather than quadratic, in the time derivatives. Hence, the momentum densities are not independent of the generalized co-ordinates, T and T^*. It can also be shown, from the variational principle in terms of the Hamiltonian density, H, after use of the four-space Green's theorem, that Hamilton's canonical equations are

$$T_{,4}\left(\frac{\partial P}{\partial T^*} - \frac{\partial P^*}{\partial T}\right) = \frac{\partial H}{\partial T^*} - \left(\frac{\partial H}{\partial T^*_{,j}}\right)_{,j} \qquad (29a)$$

$$T^*_{,4}\left(\frac{\partial P^*}{\partial T} - \frac{\partial P}{\partial T^*}\right) = \frac{\partial H}{\partial T} - \left(\frac{\partial H}{\partial T_{,j}}\right)_{,j} \qquad (29b)$$

These give no new information, however, since use of equation (22) and equation (28) in equation (29) leads back to the heat convection equation and its adjoint. This is to be expected from the discussion accompanying equation (28). Nevertheless, the fact that the adjoint momentum density is a function only of the physical temperature (and vice versa) presents some significant numerical savings, since the coefficients of a physical trial function in which they appear linearly can be solved for independently of those of the adjoint trial function.

V. REMARKS

It is seen that the restrictions in order to obtain a conservative principle, unless equation (20) can be employed, are so severe as to be infrequently met with in practice. This need not, however, be a barrier to the use of the principle, since the approximation procedure (either Ritz or Galerkin) will nevertheless normally converge satisfactorily. Barring some pathological behavior of the sought function, it is usually found that a limit appears to be approached as the

† In order to determine whether the extremal principle is minimal, cf. [4] for a brief exposition of Jacobi's theory of conjugate points.

number of trial functions is increased, even if L is not definite in sign (corresponding to a saddlepoint as the stationary point). This allows an enormous increase in versatility of the principle, since β and g, as well as the fluid velocity and thermal properties (the last requiring an obvious slight modification of the variational principle), may now be specified functions of both position and time. The nonlinear problem where the physical properties are temperature-dependent, can also be handled by an iterative method, starting with any assumed temperature distribution.

Either the Ritz or Galerkin methods [7] can be used in implementing the solution. The choice of trial functions will in some cases be improved by a foreknowledge of the form of the solution, as shown below; but in any case the use of functions belonging to an appropriate complete orthogonal set will usually have computational advantages.

Finally, some preliminary comparison between the adjoint convective variational principle with the extension of the Biot dynamical variational method developed by Nigam and Agrawal may be appropriate. One notes that the Nigam–Agrawal principle is expressed only as a variational equation, since the functional which is subject to variation is not known. The Ritz method is therefore not applicable (although the Galerkin technique can still be used). Also, solution by the dynamical principle has been demonstrated only for the case when the convective heat-transfer equation can be transformed into the heat conduction equation in a stationary medium by substitution of a new time-like variable.

VI. EXAMPLE

A simple illustrative example is now given. Consider the case where a moving slab (or fluid) passes steadily from a reservoir maintained at one temperature to another reservoir maintained at a higher temperature. Upon choosing suitable temperature and length scales, the problem can be written in dimensionless terms:

$$P\frac{\partial T}{\partial X} = \frac{\partial^2 T}{\partial X^2}; \quad T = T(X) \tag{30}$$

where P is the Peclet number, and

$$T(0) = 0; \quad T(1) = 1 \tag{31}$$

The adjoint system is then

$$-P\frac{\partial T^*}{\partial X} = \frac{\partial^2 T^*}{\partial X^2} \tag{32}$$

subject to the boundary conditions

$$T^*(0) = 0; \quad T^*(1) = 1 \tag{33}$$

The exact solutions are

$$T = \frac{e^{PX} - 1}{e^P - 1}; \quad T^* = \frac{e^{-PX} - 1}{e^{-P} - 1} \tag{34}$$

The trial functions are chosen to fit the natural boundary conditions of equation (10) and equation (14):

$$T = \frac{e^{aX} - 1}{e^a - 1}; \quad T^* = \frac{e^{bX} - 1}{e^b - 1} \tag{35}$$

Hence the surface integrals vanish identically, resulting in a variational principle of the form $\delta J_1 = 0$, where

$$J_1 = \int_0^1 \left[\frac{P}{2}\left(\frac{\partial T}{\partial X}T^* - \frac{\partial T}{\partial X}T\right) + \frac{\partial T}{\partial X}\frac{\partial T^*}{\partial X}\right] dX \tag{36}$$

Upon substituting equation (35) into equation (36), and noting that

$$\delta J_1 = \frac{\partial J_1}{\partial a}\delta a + \frac{\partial J_1}{\partial b}\delta b \tag{37}$$

the exact solutions [equation (34)] are obtained after some computation. Work is progressing on some less trivial problems, which will be reported separately.

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Résumé—Suivant une suggestion due à Morse et Feshbach, des principes variationnels adjoints sont construits pour la diffusion par convection instationnaire d'un scalaire passif, tel que la chaleur ou la masse, dans un fluide incompressible sous des conditions de généralité considérable. En ayant recours à la théorie classique des champs, des conditions suffisantes sont établies pour un principe extrémal. Un exemple simple d'illustration est donné.

Zusammenfassung—In einer inkompressiblen Flüssigkeit wurden unter ziemlich allgemeinen Bedingungen für die nichtstetige konvektive Diffusion einer passiven Skalaren, wir z.B. Wärme oder Masse nach einer Anregung, die auf Morse oder Feshbach zurückzuführen ist, beigeordnete Variationsprinzipien erstellt. Mit Hilfe der klassischen Feldtheorie werden für ein extremes Prinzip den Voraussetzungen genügende Bedingungen festgelegt. Ein einfaches anschauliches Beispiel wird angeführt.

Аннотация—По предложению Морсе и Фешбаха разработаны сопряженные вариационные принципы для нестационарной конвективной диффузии пассивной скалярной субстанции такой как тепло и масса, в несжимаемой жидкости. Обращение к классической теории полей помогло достаточные условия для экспериментального принципа. Приводится простой поясняющий пример.