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Variational Principle for Shape Design Sensitivity Analysis

Jasbir S. Arora* and J. B. Cardoso†
University of Iowa, Iowa City, Iowa 52242

In this paper, the adjoint method of design sensitivity analysis is stated as a general variational principle that is applicable to a wide range of problems. The principle gives a very simple and straightforward method of obtaining the design sensitivity expression for a functional dependent on the state fields. The sensitivity expression involves certain adjoint fields and explicit design variations of the functional and the governing equations for the primary state fields. The principle is stated in terms of an augmented functional that is defined by adding to the response functional whose sensitivity is desired, the equilibrium equation of the primary problem. Then explicit design variation of the augmented functional gives the total design variation of the response functional. Stationarity of the augmented functional with respect to the state fields defines the adjoint problem for the response functional. The principle is proved and applied to several classes of linear and nonlinear problems, such as field problems, structural problems, and dynamic response problems. It is shown that the design sensitivity expressions derived in the literature using long procedures are obtained quite routinely by use of the principle.

I. Introduction

DESIGN sensitivity analysis means the development of procedures for calculating design variations (gradient) of a functional that depends implicitly on the design variables. Implicit dependence arises because closed-form solution of the physical laws that govern the system response to inputs is generally not possible for any reasonable size practical problem. Therefore, for a given design, numerical methods must be used to determine the system response to inputs, so the explicit functional form of the response variables in terms of the design variables cannot be determined. Thus, special procedures must be derived to calculate the design gradient of a functional that depends on the response variables.

The methods of design sensitivity analysis have been developed over the last 20 years or so for different classes of engineering problems.[1,2] Two basic procedures have emerged: the direct variation (differentiation) method and the adjoint method. The finite difference method can also be used, although it is usually inefficient compared to the analytical methods. In addition, the foregoing two basic methods can be implemented in the computer using semianalytical methods. The direct variation method is quite straightforward where design variations of all governing equations for the problem are taken and solved. This way, design variations of all field variables are known, and, using these, design variation of any response functional can be evaluated. This method is simpler to implement in the computer and is suitable for some applications.[3] However, the adjoint method is suitable for several other applications. In this method, certain mathematical manipulations have been used for each class of problem to develop an analytical expression for calculating the design variations (gradient).

It turns out that the adjoint method of sensitivity analysis can be transcribed into the form of a generalized variational principle. The principle gives a straightforward way of obtaining the gradient formula and defining the adjoint problem. The purposes of this paper are to state and prove this principle and to demonstrate it on several classes of problems. Fundamental work in this regard was reported recently for linear problems.[4-6] More recently, a similar procedure was applied to thermal problems.[7,8] Material presented in these references will augment the present paper. The principle is applicable to linear as well as nonlinear problems. This is demonstrated by applying it to linear and nonlinear field problems, structural problems, and dynamic problems.

II. Variational Principle

The problem is to derive an expression for design variation of a general functional that depends on design varriables and state variables. For presentation of a universal procedure that can be used for any type of problem, consider a general functional expressed symbolically as

$$\psi(\boldsymbol{b},\boldsymbol{u}) \tag{1}$$

Where $\boldsymbol{b} \in R^k$ is a design variable vector and $\boldsymbol{u} = \boldsymbol{u}[\boldsymbol{x}(\boldsymbol{b}),\boldsymbol{b}]$ is a field variable vector containing such quantities as stress, strain, displacement, pressure, and reaction force fields. For most applications, the functional ψ depends implicitly on the design variables $\boldsymbol{b}$, since $\boldsymbol{u}$ depends implicitly on design through a state equation written symbolically as

$$W(\boldsymbol{b},\boldsymbol{u}) = 0 \tag{2}$$

Equation (2) may represent a matrix equation for finite dimensional systems or a set of differential equations for the continuum models. The exact form of the equation will become transparent when different applications are considered later in the paper.

Direct design variation of the functional in Eq. (1) for a finite dimensional system can be written as

$$\bar{\delta}\psi \equiv \frac{\mathrm{d}\psi^T}{\mathrm{d}\boldsymbol{b}}\,\delta\boldsymbol{b} = \left(\frac{\partial\psi^T}{\partial\boldsymbol{b}} + \frac{\partial\psi^T}{\partial\boldsymbol{u}}\frac{\mathrm{d}\boldsymbol{u}}{\mathrm{d}\boldsymbol{b}}\right)\delta\boldsymbol{b} \tag{3}$$

where $\bar{\delta}$ represents the total design variation operator and $\boldsymbol{u}$ is an n dimensional vector. For many applications, it is inefficient to compute directly the $n \times k$ matrix $\mathrm{d}\boldsymbol{u}/\mathrm{d}\boldsymbol{b}$ appearing in Eq. (3). The idea of the adjoint method is to avoid this computation.

A. Design Sensitivity Principle

To state the adjoint method as a variational principle, define an augmented functional by adding to the functional whose

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*Professor, College of Engineering, Optimal Design Laboratory.
†Optimal Design Laboratory; currently at Universidade Técnica de Lisboa, Portugal.

sensitivity is desired the governing state equation containing a free variable as

$$L(\boldsymbol{b},\boldsymbol{u},\boldsymbol{u}^a) = \psi(\boldsymbol{b},\boldsymbol{u}) + W^a(\boldsymbol{b},\boldsymbol{u},\boldsymbol{u}^a) \text{ with } W^a = [\boldsymbol{u}^a, W(\boldsymbol{b},\boldsymbol{u})] \tag{4}$$

where $\boldsymbol{u}^a$ is a kinematically admissible but otherwise unspecified adjoint field that needs to be determined and (f,g) denotes the inner product. Note that $W^a = 0$ represents a weak form of the state equation. Let the adjoint field $\boldsymbol{u}^a$ be determined such that the augmented functional L in Eq. (4) is stationary with respect to the variations of the primary state fields; i.e., let

$$\tilde{\delta} L = 0 \tag{5}$$

where $\tilde{\delta}$ represents variations (partial derivatives) with respect to the primary state fields. Then it is true that the total design variation of the functional ψ in Eq. (1) is given as the explicit design variation (partial derivative) of the augmented functional in Eq. (4), i.e.,

$$\bar{\delta}\psi = \bar{\bar{\delta}} L \tag{6}$$

where $\bar{\bar{\delta}}$ denotes the explicit design variation operator.

B. Proof

Proof of the principle is quite straightforward. Total design variation of the functional (4) gives

$$\bar{\delta} L = \bar{\delta}\psi + \bar{\delta} W^a \tag{7}$$

But $\bar{\delta} W^a = (\bar{\delta}\boldsymbol{u}^a, W) + (\boldsymbol{u}^a, \bar{\delta} W)$. If $\bar{\delta}\boldsymbol{u}^a$ is also selected to be kinematically admissible, then $(\bar{\delta}\boldsymbol{u}^a, W) = 0$. In addition, the equilibrium is required to hold at the current design and the varied design, i.e., $(\boldsymbol{u}^a, W) = 0$ and $(\boldsymbol{u}^a, W + \bar{\delta} W) = 0$. Thus, Eq. (7) reduces to

$$\bar{\delta}\psi = \bar{\delta} L \tag{8}$$

Now $\bar{\delta} L$ can be written as

$$\bar{\delta} L = \bar{\bar{\delta}} L + \tilde{\delta} L \tag{9}$$

But the principle requires L to be stationary with respect to the primary state fields, i.e., $\tilde{\delta} L = 0$ [Eq. (5)]. Hence, Eqs. (8), (9), and (5) prove that $\bar{\delta}\psi = \bar{\bar{\delta}} L$. The requirement $\tilde{\delta} L = 0$ gives governing equations that must be solved to determine $\boldsymbol{u}^a$. This auxiliary problem for $\boldsymbol{u}^a$ is sometimes called the "virtual problem," the "imaginary problem," the "pseudoproblem," or the "adjoint problem." Only the field $\boldsymbol{u}^a$ determined by solving this auxiliary problem can be used to obtain $\bar{\delta}\psi = \bar{\bar{\delta}} L$.||

It can be seen that the principle can be very useful in obtaining design sensitivity expressions for different classes of problems in a very simple and straightforward manner. It is important to note that other state equations such as the constitutive laws and the strain displacement equations can also be added to the augmented functional of Eq. (4) by introducing adjoint variables for the them. The foregoing procedure will generate governing equations for these additional adjoint variables. In the sequel, we consider field problems, structural problems, and dynamic problems to obtain design sensitivity expressions for the appropriate response functionals to demonstrate use of the principle.

III. Field Problems

Many problems from different branches of science and engineering have a common characteristic of being governed by similar partial differential equations. These are called the field problems, such as electric and heat conduction, seepage, fluid flow, fluid-film lubrication, torsion, magnetostatics, and diffusion of porous media.[9,10] Finite element techniques for analysis of such problems are under active research and development.[11-13]

Derivation of a design sensitivity expression for a response functional related to field problems is considered in this section. Both the variational form of the governing equation as well as its differential form are considered for linear and nonlinear steady-state problems. A direct application of the variational design sensitivity principle gives the design sensitivity expression as well as definition of the adjoint problem. Analytical examples showing application of the expression have also been presented.[14,15] Design sensitivity analysis of thermal systems were also recently considered in Refs. 7, 8, and 16.

A. Nonlinear Field Problem

Suppose a field variable ϕ is to be found in a domain of volume V bounded by a surface S (Fig. 1). For steady-state problems, the governing equations are expressed at the current state as

$$-\nabla\cdot\boldsymbol{f} + (P\phi + Q) = 0; \qquad \boldsymbol{f} = -\boldsymbol{K}\,\nabla\phi \text{ in } V \tag{10}$$

$$\phi = \phi^0, \text{ on } S_\phi$$

$$-\boldsymbol{f}\cdot\boldsymbol{n} + (p^0\phi + q^0) = 0, \text{ on } S_q \tag{11}$$

where $\boldsymbol{f}$ is the flux, ∇ is the gradient operator with respect to the space variables, $\boldsymbol{x}\cdot\boldsymbol{y}$ represents the proper inner product of vectors and matrices, $\boldsymbol{K} \equiv \boldsymbol{K}(\phi)$ is a matrix of material parameters, $\boldsymbol{n}$ is the unit normal to the boundary, $(P\phi + Q)$ is a generalized specific domain flux, $(p^0\phi + q^0)$ is a generalized specified flow input to the surface, and $S = S_\phi \cup S_q$, S_ϕ being the part of the boundary where the field ϕ is prescribed and S_q being the part of the boundary where the flux is prescribed. Note that $\boldsymbol{K}$ is a symmetric operator, and $S_q = S_f \cup S_c \cup S_r$ where S_f is the part of the boundary with a specified flux $q^0 = f^0$, S_c is the convective part, and S_r is its radiation part. Also, $p^0 = 0$ on S_f, $p^0 \equiv k_c(\phi)$ and $q^0 \equiv -k_c\phi_s$ on S_c, and $p^0 = k_r(\phi)$ and $q^0 \equiv -k_r(\phi)$ on S_r, where k_c and k_r are, respectively, the convection and radiation coefficients of the medium surrounding the domain and ϕ_s is the value of the field in that medium. The problem just considered is a physically nonlinear problem, where all the material parameters depend on the state ϕ.

The variational (weak) form of Eqs. (10) and (11) is

$$\delta W \equiv -\int \boldsymbol{f}\cdot\delta(\nabla\phi)\,\mathrm{d}V - \int (P\phi + Q)\delta\phi\,\mathrm{d}V + \int (p^0\phi + q^0)\delta\phi\,\mathrm{d}S_q = 0 \tag{12}$$

where the variations of the state fields are arbitrary but kinematically admissible. The quantities $\boldsymbol{K}$, P, Q, p^0, and q^0 may depend on the state field ϕ, so Eqs. (10–12) are nonlin-

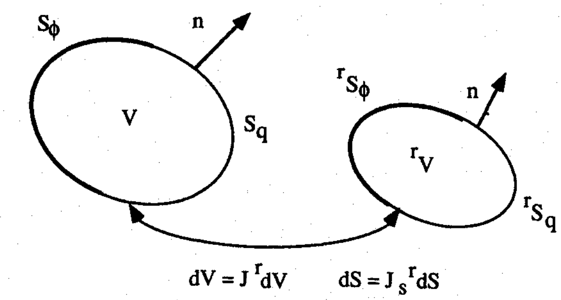

Fig. 1 Problem domain and fixed reference domain.

ear. Using the concept of reference (control) volume,[17-20] one transforms all of the configurations for analysis and design to a fixed reference domain (Fig. 1) that remains unchanged during analysis and design. Let ξ_i be the coordinates in the fixed reference domain with volume ${}^rV$ and surface ${}^rS$ that do not change with design variations. With respect to the reference domain, Eq. (12) for the primary state fields is transformed as

$$\delta W \equiv - \int f \cdot \delta(\nabla\phi) J \, {}^r\mathrm{d}V - \int (P\phi + Q)\delta\phi J \, {}^r\mathrm{d}V + \int (p^0\phi + q^0)\delta\phi J_s \, {}^r\mathrm{d}S_q = 0 \tag{13}$$

where

$$\nabla\phi = X^{-T}({}_r\nabla\xi) \qquad \mathrm{d}V = J \, {}^r\mathrm{d}V \qquad \mathrm{d}S = J_s \, {}^r\mathrm{d}S \tag{14}$$

$$X = [\partial x_i/\partial \xi_j], \qquad J = |X|, \qquad J_s = J \, \|X^{-T}\boldsymbol{n}\| \tag{15}$$

and $\boldsymbol{n}$ now represents normal to the reference domain boundary. In the foregoing equations, superscript and subscript r refers to the coordinates of the reference domain, X is the Jacobian matrix of the transformation, J is the Jacobian determinant, and J_s is the area metric.

B. Design Sensitivity Analysis

The design of systems governed by field equations (10–15) requires the evaluation of some performance functionals that depend on the field variable, its gradient, and the flux or flow in the system. In a generalized form, a performance functional is expressed as

$$\psi = \int G(f, \nabla\phi, \phi, \boldsymbol{b}) \, \mathrm{d}V(\boldsymbol{b}) + \int h(\phi, \boldsymbol{b}) \, \mathrm{d}S_q(\boldsymbol{b}) \tag{16}$$

where $\boldsymbol{b}$ is the design variable vector and $Z \equiv (f, \nabla\phi, \phi)$ defines the state space. After transformation to the reference domain, Eq. (16) becomes

$$\psi = \int G(f, \nabla\phi, \phi, \boldsymbol{b}) J(\boldsymbol{b}) \, {}^r\mathrm{d}V + \int h(\phi, \boldsymbol{b}) J_s(\boldsymbol{b}) \, {}^r\mathrm{d}S_q \tag{17}$$

where now the domain is free of design and integrands are functions of the reference coordinates. To apply the variational principle of design sensitivity analysis, one can define the augmented functional of Eq. (4) with W^a given as

$$W^a \equiv - \int f \cdot \nabla\phi^a J \, {}^r\mathrm{d}V - \int (P\phi + Q)\phi^a J \, {}^r\mathrm{d}V + \int (p^0\phi + q^0)\phi^a J_s \, {}^r\mathrm{d}S_q = 0 \tag{18}$$

Equation (18) gives a weak form of the governing equation for the primary problem in which the primary virtual state fields $\delta\phi$ and $\delta(\nabla\phi)$ have been replaced by the yet unknown adjoint fields ϕ^a and $\nabla\phi^a$ with

$$\nabla\phi^a = X^{-T}({}_r\nabla\phi^a) \tag{19}$$

Since ϕ^a and $\nabla\phi^a$ are kinematically admissible and compatible, they can be used as virtual fields for the primary problem. Substituting Eqs. (17) and (18) into Eq. (4), we get

$$L = \int [G - f \cdot \nabla\phi^a - (P\phi + Q)\phi^a] J \, {}^r\mathrm{d}V + \int [h + (p^0\phi + q^0)\phi^a] J_s \, {}^r\mathrm{d}S_q \tag{20}$$

According to the sensitivity principle, total design variation of the functional ψ is given as the explicit design variation of the augmented functional L, i.e., $\bar{\delta}\psi = \bar{\bar{\delta}}L$,

$$\begin{aligned} \bar{\delta}\psi = & \int [G - f \cdot \nabla\phi^a - (P\phi + Q)\phi^a] \bar{\bar{\delta}} J \, {}^r\mathrm{d}V \\ & + \int [h + (p^0\phi + q^0)\phi^a] \bar{\bar{\delta}} J_s \, {}^r\mathrm{d}S_q \\ & + \int [G_{,b} \cdot \delta\boldsymbol{b} + G_{,f} \cdot \bar{\bar{\delta}} f + G_{,\nabla\phi} \cdot \bar{\bar{\delta}}(\nabla\phi) - \bar{\bar{\delta}} f \cdot \nabla\phi^a \\ & - f \cdot \bar{\bar{\delta}}(\nabla\phi^a) - (\bar{\bar{\delta}} P\phi + \bar{\bar{\delta}} Q)\phi^a] J \, {}^r\mathrm{d}V \\ & + \int [h_{,b} \cdot \delta\boldsymbol{b} + (\bar{\bar{\delta}} p^0\phi + \bar{\bar{\delta}} q^0)\phi^a] J_s \, {}^r\mathrm{d}S_q \end{aligned} \tag{21}$$

Explicit design variation of f in Eq. (10) gives

$$\bar{\bar{\delta}} f = -\boldsymbol{K} \, \bar{\bar{\delta}}(\nabla\phi) - \bar{\bar{\delta}}\boldsymbol{K} \, \nabla\phi \tag{22}$$

The Fourier's law for the adjoint problem gets defined as follows when various terms are collected in Eq. (21):

$$f^a = -\boldsymbol{K}[\nabla\phi^a - G_{,f}] - G_{,\nabla\phi} \tag{23}$$

This law will also be used in defining the adjoint problem later. Substituting Eqs. (22) and (23) into Eq. (21) and collecting terms, we obtain the final sensitivity expression as

$$\begin{aligned} \bar{\delta}\psi = & \int \{[(\nabla\phi^a - G_{,f}) \cdot \nabla\phi \bar{\bar{\delta}}\boldsymbol{K} - f^a \cdot \bar{\bar{\delta}}(\nabla\phi) \\ & - f \cdot \bar{\bar{\delta}}(\nabla\phi^a) - (\bar{\bar{\delta}} P\phi + \bar{\bar{\delta}} Q)\phi^a + G_{,b} \cdot \delta\boldsymbol{b}] J \\ & + [G - f \cdot \nabla\phi^a - (P\phi + Q)\phi^a] \bar{\bar{\delta}} J\} \, {}^r\mathrm{d}V \\ & + \int \{[(\bar{\bar{\delta}} p^0\phi + \bar{\bar{\delta}} q^0)\phi^a + h_{,b} \cdot \delta\boldsymbol{b}] J_s \\ & + [h + (p^0\phi + q^0)\phi^a] \bar{\bar{\delta}} J_s\} \, {}^r\mathrm{d}S_q \end{aligned} \tag{24}$$

According to Eq. (5), the implicit variation (i.e., variation with respect to the state fields) of the augmented functional L should be set to zero, giving

$$\begin{aligned} & \int [G_{,\nabla\phi} \cdot \tilde{\delta}(\nabla\phi) + G_{,\phi} \cdot \tilde{\delta}\phi + (G_{,f} - \nabla\phi^a) \cdot \tilde{\delta} f \\ & - f \cdot \tilde{\delta}(\nabla\phi^a) - (P\phi + Q)_{,\phi} \tilde{\delta}\phi \, \phi^a \\ & - (P\phi + Q)\tilde{\delta}\phi^a] J \, {}^r\mathrm{d}V + \int [h_{,\phi} \cdot \tilde{\delta}\phi \\ & + (p^0\phi + q^0)_{,\phi} \tilde{\delta}\phi\phi^a + h \\ & + (p^0\phi + q^0)\tilde{\delta}\phi^a] J_s \, {}^r\mathrm{d}S_q = 0 \end{aligned} \tag{25}$$

Substituting $\tilde{\delta} f$ from Eq. (10) into Eq. (25), collecting terms and using the definition of Fourier's law from Eq. (23), we get the adjoint problem as

$$\begin{aligned} & \int \{-f^a \cdot \tilde{\delta}(\nabla\phi) + (\nabla\phi^a - G_{,f})\boldsymbol{K}_{,\phi} \nabla\phi \tilde{\delta}\phi\} J \, {}^r\mathrm{d}V \\ & = \int \{(P\phi + Q)_{,\phi}\phi^a - G_{,\phi}\} \tilde{\delta}\phi J \, {}^r\mathrm{d}V \\ & - \int \{(p^0\phi + q^0)_{,\phi}\phi^a + h_{,\phi}\} \tilde{\delta}\phi J_s \, {}^r\mathrm{d}S_q \end{aligned} \tag{26}$$

which is obtained after dropping the expression

$$\int f \cdot \tilde{\delta}(\nabla\phi^a) J \, {}^r\mathrm{d}V + \int (P\phi + Q)\tilde{\delta}\phi^a J \, {}^r\mathrm{d}V - \int (p^0\phi + q^0)\tilde{\delta}\phi^a J_s \, {}^r\mathrm{d}S_q$$

since they constitute the governing equation of the primary problem. In Eq. (26), $\delta\phi$ can replace $\bar{\delta}\phi$ since $\bar{\delta}\phi$ is a kinematically admissible variation of the primary field. Equation (26) has the same material parameter matrix as the tangential material parameter matrix of the original or primary problem. Its input consists of initial adjoint flux $KG_{,f}$, initial adjoint field gradient $G_{,\nabla\phi}$, distributed volumic flux ($P^a\phi^a + Q^a$), and flow input to the surface ($p^{a0}\phi^a + q^{a0}$), where $Q^a = -G_{,\phi}$, $P^a = (P\phi + Q)_{,\phi}$, $q^{a0} = h_{,\phi}$, $p^{a0} = (p^0\phi + q^0)_{,\phi}$, are dependent on the primary state fields.

IV. Linear Structural Problems

Design sensitivity analysis of linear structural problems has been developed since the early 1970s. Discrete and continuum models as well as shape and nonshape problems have been addressed. For continuum models, two methods—the control volume and material derivative approaches—have been developed. In the present section, the design sensitivity analysis principle is used to treat both the discrete and the continuum models.

A. Finite Dimensional Formulation

In the finite dimensional form, the equilibrium equation for the structure is given as

$$K(b)U = R(b) \tag{27}$$

where K is an $n \times n$ structural stiffness matrix, b is a k-dimensional design variable vector, U is the n-dimensional nodal displacement vector, and $R(b)$ is the equivalent nodal load vector. Equation (27) is obtained when standard finite element procedures are used to discretize the continuum. Let the function whose sensitivity is desired be given as $\psi(b,U)$. To use the design sensitivity analysis principle, define the augmented functional as

$$L = \psi(b,U) + W^a \text{ with } W^a = U^{aT}(R(b) - K(b)U) \tag{28}$$

where U^a is a vector that needs to be determined. According to Eq. (6) of the principle, total derivative of ψ is equal to the partial derivative of L, i.e.,

$$\frac{d\psi}{db} = \frac{\partial\psi}{\partial b} + \frac{\partial}{\partial b}(R(b) - K(b)U)^T U^a \tag{29}$$

which is the same as in Refs. 21 and 22 and many other references in the literature. Also, the augmented functional L is required to be stationary with respect to the state variables U, i.e., $\partial L/\partial U = 0$ which gives

$$\frac{\partial\psi}{\partial U} - K^T(b)U^a = 0 \quad \text{or} \quad K(b)U^a = \frac{\partial\psi}{\partial U} \tag{30}$$

which is the adjoint equation that determines U^a for use in Eq. (29).

The adjoint displacements U^a are interpreted as the Lagrange multipliers for the state equation.[6] This interpretation can be useful in practical implementation of design sensitivity analysis as well as other practical applications.

B. Continuum Formulation: Control Volume Approach

The virtual work equation governing the equilibrium state of a continuum is given as

$$\int \sigma_{ij}\delta e_{ij}\, dV - \int f_i\delta u_i\, dV - \int T_i^0\delta u_i\, dS_T - \int T_i\delta u_i^0\, dS_u = 0 \tag{31}$$

where σ_{ij} is the Cauchy stress tensor, e_{ij} is the infinitesimal strain tensor, f_i is the body force field, T_i^0 is the specified surface traction on S_T, and T_i is the reaction traction on S_u, u_i^0 is the specified displacement on S_u, u_i is the displacement field, V is the volume occupied by structure, S_T is the traction specified surface, S_u is the displacement specified surface, and δ represents arbitrary but kinematically admissible variation. The last integral in Eq. (31) is usually zero, but it is included so that design sensitivity of the reaction traction T_i can be calculated.

The strain-displacement relationship and its arbitrary variation are given as

$$e_{ij} = \tfrac{1}{2}(u_{i,j} + u_{j,i}); \qquad \delta e_{ij} = \tfrac{1}{2}(\delta u_{i,j} + \delta u_{j,i}) \tag{32}$$

where $u_{i,j} = \partial u_i/\partial x_j$. The linear stress-strain law is given as

$$\sigma_{ij} = D_{ijk\ell}e_{k\ell} \tag{33}$$

where $D_{ijk\ell}$ is the material modulus tensor.

In the control volume concept, all of the field variables and the integrals are transformed to a fixed reference domain by using an independent variable transformation as in the previous section. Substituting the transformations to the reference domain in Eqs. (16) and (17), Eqs. (31) and (32) become

$$\int (\sigma_{ij}\delta e_{ij} - f_i\delta u_i)J\, {}^r dV - \int T_i^0\delta u_i J_s\, {}^r dS_T - \int T_i\delta u_i^0 J_s\, {}^r dS_u = 0 \tag{34}$$

$$e_{ij} = \tfrac{1}{2}[\xi_{k,i}u_{j;k} + u_{i;k}\xi_{k,j}] \qquad \delta e_{ij} = [\delta u_{i;k}\xi_{k,j} + \delta u_{j;k}\xi_{k,i}] \tag{35}$$

where $\xi_{k,i} = \partial\xi_k/\partial x_i$ and $u_{j;k} = \partial u_j/\partial\xi_k$.

Constraints for the structure are imposed on stresses, strains, displacements, and reaction forces. These constraints may be imposed at a particular point in the structure or over a subdomain and, after transformation to the reference domain, can be written in general as

$$\psi = \int G(\sigma_{ij},e_{ij},u_i,b)J\, {}^r dV + \int g(u_i^0,T_i,b)J_s\, {}^r dS_u + \int h(u_i,T_i^0,b)J_s\, {}^r dS_T \tag{36}$$

This functional depends explicitly as well as implicitly on the design variables.

To use the principle, one replaces the arbitrary state fields in the virtual work expression (34) by the adjoint fields that will be determined later. Thus, the final weak form of the governing equation for use in Eq. (4) is given as follows:

$$W^a \equiv \int (-\sigma_{ij}e_{ij}^a + f_iu_i^a)J\, {}^r dV + \int T_i^0u_i^aJ_s\, {}^r dS_T + \int T_iu_i^{a0}J_s\, {}^r dS_u = 0 \tag{37}$$

where e_{ij}^a is given using δe_{ij} in Eq. (35) as

$$e_{ij}^a = \tfrac{1}{2}[u_{i;k}^a\xi_{k,j} + u_{i;k}^a\xi_{k,i}] \tag{38}$$

and u_i^{a0} is a specified displacement (to be defined later). The augmented functional of Eq. (4) is defined as $L = \psi + W^a$, and, according to the principle, the total design variation of the constraint functional is given as the explicit design variation of the functional L as

$$\bar{\delta}\psi = \bar{\bar{\delta}}L = \bar{\bar{\delta}}\psi + \bar{\bar{\delta}}W^a \tag{39}$$

The explicit design variation $\bar{\bar{\delta}}\psi$ is given from Eq. (36) as

$$\bar{\bar{\delta}}\psi = \int \bar{\bar{\delta}}(GJ)\,{}^r\mathrm{d}V + \int \bar{\bar{\delta}}(gJ_s)\,{}^r\mathrm{d}S_u + \int \bar{\bar{\delta}}(hJ_s)\,{}^r\mathrm{d}S_R \tag{40}$$

$$\bar{\bar{\delta}}G = G_{,\sigma_{ij}}\bar{\bar{\delta}}\sigma_{ij} + G_{,e_{ij}}\bar{\bar{\delta}}e_{ij} + G_{,b_i}\,\delta b_i \tag{41}$$

$$\bar{\bar{\delta}}g = g_{,u_i}\bar{\bar{\delta}}u_i^0 + g_{,T_i}\bar{\bar{\delta}}T_i + g_{,b_i}\,\delta b_i \tag{42}$$

$$\bar{\bar{\delta}}h = h_{,u_i}\bar{\bar{\delta}}u_i + h_{,T_i}\bar{\bar{\delta}}T_i^0 + h_{,b_i}\delta b_i \tag{43}$$

$\bar{\bar{\delta}}W^a$ is given from Eq. (33) as

$$\bar{\bar{\delta}}W^a = \bar{\bar{\delta}}\int - \sigma_{ij}e_{ij}^aJ\,{}^r\mathrm{d}V + \bar{\bar{\delta}}\int f_iu_i^aJ\,{}^r\mathrm{d}V + \bar{\bar{\delta}}\int T_i^0u_i^aJ_s\,{}^r\mathrm{d}S_T + \bar{\bar{\delta}}\int T_iu_i^{a0}J_s\,{}^r\mathrm{d}S_u \tag{44}$$

To calculate the design sensitivity using Eq. (39), the adjoint fields are needed. According to the design sensitivity analysis principle, the governing equilibrium equation for the adjoint structure can be obtained by requiring the implicit variation of the augmented functional in Eq. (4) to vanish; i.e.,

$$\tilde{\delta}L = 0 \quad \text{or} \quad \tilde{\delta}\psi + \tilde{\delta}W^a = 0 \tag{45}$$

To impose the condition in Eq. (45), we write $\tilde{\delta}\sigma$ and $\tilde{\delta}W^a$ using Eqs. (36) and (37) as

$$\tilde{\delta}\psi = \int (G_{,\sigma_{ij}}\tilde{\delta}\sigma_{ij} + G_{,e_{ij}}\tilde{\delta}e_{ij} + G_{,u_i}\tilde{\delta}u_i)J\,{}^r\mathrm{d}V + \int g_{,T_i}\tilde{\delta}T_iJ_s\,{}^r\mathrm{d}S_u + \int h_{,u_i}\tilde{\delta}u_iJ_s\,{}^r\mathrm{d}S_T \tag{46}$$

$$\tilde{\delta}W^a = \left\{\int(-\sigma_{ij}\tilde{\delta}e_{ij}^a + f_i\tilde{\delta}u_i^a)J\,{}^r\mathrm{d}V + \int T_i^0\tilde{\delta}u_i^aJ_s^r\,\mathrm{d}S_T\right\} - \int\tilde{\delta}\sigma_{ij}e_{ij}^aJ\,{}^r\mathrm{d}V + \int\tilde{\delta}T_iu_i^0J_s\,{}^r\mathrm{d}S_u \tag{47}$$

where $\tilde{\delta}T_i = 0$ on S_T and $u_i^a = u_i^{a0}$ on S_u have been used. In Eq. (47), the expression within the braces represents equilibrium equation for the primary structure, so it vanishes and $\tilde{\delta}W^a$ reduces to

$$\tilde{\delta}W^a = -\int\tilde{\delta}\sigma_{ij}e_{ij}^aJ\,{}^r\mathrm{d}V + \int\tilde{\delta}T_iu_i^{a0}J_s\,{}^r\mathrm{d}S_u \tag{48}$$

Referring to Eq. (46), let us define the following quantities for the adjoint structure:

Initial Strain: $e_{ij}^{aI} = G_{,\sigma_{ij}}$ in V

Initial Stress: $\sigma_{ij}^{aI} = G_{,e_{ij}}$ in V

Body Force: $f_i^a = G_{,u_i}$ in V

Boundary Displacement: $u_i^{a0} = -g_{,T_i}$ on S_u

Specified Traction: $T_i^{a0} = h_{,u_i}$ on S_T (49)

Substituting Eqs. (46), (48), and (49) into Eq. (45), we have

$$\int(e_{ij}^{aI}\tilde{\delta}\sigma_{ij} + \sigma_{ij}^{aI}\tilde{\delta}e_{ij} + f_i^a\tilde{\delta}u_i)J\,{}^r\mathrm{d}V - \int u_i^{a0}\tilde{\delta}T_iJ_s\,{}^r\mathrm{d}S_u + \int T_i^{a0}\tilde{\delta}u_iJ_s\,{}^r\mathrm{d}S_T - \int\tilde{\delta}\sigma_{ij}e_{ij}^aJ\,{}^r\mathrm{d}V + \int\tilde{\delta}T_iu_i^{a0}J_s\,{}^r\mathrm{d}S_u = 0$$

Collecting terms and using $\tilde{\delta}\sigma_{ij} = \mathrm{D}_{ijk\ell}\tilde{\delta}e_{k\ell}$, we have

$$\int[-(\mathrm{D}_{ijk\ell}(e_{ij}^a - e_{ij}^{aI}) - \sigma_{k\ell}^{aI})\tilde{\delta}e_{k\ell} + f_i^a\tilde{\delta}u_i]J\,{}^r\mathrm{d}V + \int T_i^{a0}\tilde{\delta}u_iJ_s\,{}^r\mathrm{d}S_T = 0 \tag{50}$$

If we define the stress-strain law for the adjoint structure as

$$\sigma_{ij}^a = \mathrm{D}_{ijk\ell}(e_{k\ell}^a - e_{k\ell}^{aI}) - \sigma_{ij}^{aI} \tag{51}$$

where $\mathrm{D}_{ijk\ell}$ is assumed to be symmetric, then Eq. (50) becomes

$$\int(-\sigma_{ij}^a\tilde{\delta}e_{ij} + f_i^a\tilde{\delta}u_i)J\,{}^r\mathrm{d}V + \int T_i^{a0}\tilde{\delta}u_iJ_s\,{}^r\mathrm{d}S_T = 0 \tag{52}$$

Equation (52) represents the governing equilibrium equation for the adjoint structure because $\tilde{\delta}u_i$ can be considered as arbitrary with $\tilde{\delta}e_{ij}$ to be compatible with it.

The adjoint method is now summarized as follows: use Eqs. (33–35) to determine the primary field variables, use Eqs. (38), (51), and (52) to determine the adjoint fields, calculate explicit design variations of the primary stresses and strains given in Eqs. (33) and (34), respectively, calculate explicit design variations of the adjoint stresses and strains given in Eqs. (51) and (38), respectively, and then use Eq. (36) to calculate the final design sensitivity coefficients.

C. Continuum Formulation: Material Derivative Approach

The material derivative approach of structural design sensitivity analysis has been developed over the last 10 yr.[23–31] The method has been developed from several different points of view. A variety of notations has been used, and varying degrees of mathematical sophistications and arguments have been used to derive several different forms of the design sensitivity expression. Also, different procedures have been used to obtain the final expression. Here we will derive a sensitivity expression using the material derivative concept of continuum mechanics and variation of integrals over a variable domain discussed in the calculus of variations. Other forms of the expressions can also be derived.[32] In the sequel, all of the derivatives are assumed to exist, with domains simply connected and the surfaces smooth. This is done to keep the presentation as simple as possible. Nonsmooth surfaces and interface problems have been addressed in the literature.

Before deriving the sensitivity expressions, the basic material derivative expression that is useful in various derivations is given. Consider a domain Ω occupying a volume V and bounded by the surface S. Let only one parameter b define the transformation to the modified domain $\overline{\Omega}$ as $\xi_i = \xi_i(\boldsymbol{x},\underline{b})$ where x_i are coordinates in Ω and ξ_i are coordinates in $\overline{\Omega}$. Thinking of b as a time-like parameter, a design velocity field is defined as $v_i(\xi,b) = \partial\xi_i/\partial b$. In a neighborhood of $b = 0$, linear Taylor's expansion gives $\xi_i(\boldsymbol{x},b) = x_i + bv_i(\boldsymbol{x})$ where $\boldsymbol{v}(\boldsymbol{x}) = \boldsymbol{v}(\xi,0) = \boldsymbol{v}(\boldsymbol{x},0)$ and $\xi(\boldsymbol{x},0) = \boldsymbol{x}$. Now, the *material derivative* of a scalar field variable $z(\boldsymbol{x})$ is defined as

$$\dot{z} = z'(\boldsymbol{x}) + \nabla z(\boldsymbol{x})\cdot\boldsymbol{v}(\boldsymbol{x}), \quad \text{or} \quad \dot{z} = z' + z_{,k}v_k \tag{53}$$

where $z'(\boldsymbol{x})$ is the local derivative of z at $\boldsymbol{x}$, and a dot over a variable denotes the material derivative. A *material derivative operator* that can be used in general is defined as

$$(\dot{\ }) = (\ )' + \boldsymbol{v}\cdot\nabla(\ ), \quad \text{or} \quad (\dot{\ }) = (\ )' + v_k(\ )_{,k} \tag{54}$$

Note that the *convective term* $\boldsymbol{v}\cdot\nabla(\ )$ is an explicit design derivative. This fact will be utilized in the following derivations.

To derive the design sensitivity expression, one defines the augmented functional $L = \psi + W^a$ of Eq. (4) using Eqs. (36)

and (37) in the material domain as

$$L = \int (G - \sigma_{ij}e^a_{ij} + f_i u^a_i)\, dV + \int (g + T_i u^{a0}_i)\, dS_u + \int (h + T^0_i u^a_i)\, dS_T = \int \overline{G}\, dV + \int \overline{g}\, dS_u + \int \overline{h}\, dS_T \tag{55}$$

where

$$\overline{G} = G - \sigma_{ij}e^a_{ij} + f_i u^a_i$$

$$\overline{g} = g + T_i u^{a0}_i; \qquad \overline{h} = h + T^0_i u^a_i \tag{56}$$

Take the variation of Eq. (55) with respect to the state fields and set the terms involving the local design variation of the state fields to zero:

$$\int [(G_{,\sigma_{ij}}\sigma'_{ij} + G_{,e_{ij}}e'_{ij} + G_{,u_i}u'_i) - (\sigma'_{ij}e^a_{ij} + \sigma_{ij}e^{a\prime}_{ij} - f_i u^{a\prime}_i)]\, dV + \int [h_{,u_i}u'_i + T^0_i u^{a\prime}_i] + \int [g_{,T_i}T'_i + T'_i u^{a0}_i] = 0 \tag{57}$$

Substitute Eqs. (49) and the adjoint stress-strain law of Eq. (51) into Eq. (57) to obtain

$$\left\{\int (-\sigma^a_{ij}e'_{ij} + f^a_i u'_i)\, dV + \int T^{a0}_i u'_i\, dS_T\right\} + \left\{\int (-\sigma_{ij}e^{a\prime}_{ij} + f_i u^{a\prime}_i)\, dV + \int T^0_i u^{a\prime}_i\, dS_T\right\} - \int u^{a0}_i T'_i\, dS_u + \int T'_i u^{a0}_i\, dS_u = 0 \tag{58}$$

The expression in the second pair of braces vanishes because it represents the equilibrium equation for the primary structure, and the last two terms cancel with each other; thus, Eq. (58) reduces to

$$\int (-\sigma^a_{ij}e'_{ij} + f^a_i u'_i)\, dV + \int T^{a0}_i u'_i\, dS_T = 0 \tag{59}$$

which is the equilibrium equation that determines the adjoint displacement field.

To obtain the material derivative of ψ, take the derivative of the augmented functional in Eq. (55) and neglect the implicit derivative terms that have been already set to zero in Eq. (57):

$$\dot{\psi} = \int (G - \sigma_{ij}e^a_{ij} + f_i u^a_i)\dot{\overline{dV}} + \int [G_{,b} + (G_{,\sigma_{ij}}\nabla\sigma_{ij}\cdot v + G_{,e_{ij}}\nabla e_{ij}\cdot v + G_{,u_i}\nabla u_i\cdot v) - \nabla(\sigma_{ij}e^a_{ij})\cdot v + \dot{f}_i u^a_i + f_i(\nabla u^a_i\cdot v)]\, dV + \int [g_{,b} + g_{,T_i}\nabla T_i\cdot v + g_{,u_i}\dot{u}^0_i + (\nabla T_i\cdot v)u^{a0}_i + T_i\dot{u}^{a0}_i]\, dS_u + \int (g + T_i u^{a0}_i)\dot{\overline{dS_u}} + \int [h_{,b} + h_{,u_i}\nabla u_i\cdot v + T^0_i\nabla u^a_i\cdot v + \dot{T}^0_i u^a_i + h_{,T_i}\dot{T}^0_i]\, dS_T + \int (h + T^0_i u^a_i)\dot{\overline{dS_T}} \tag{60}$$

$$\dot{\overline{dV}} = v_{k,k}\, dV; \qquad \dot{\overline{dS}} = (\delta_{k\ell} - n_k n_\ell)v_{k,\ell}\, dS \tag{61}$$

This equation can be used as is, or it can be reduced to the ones derived in the literature.[23-32]

V. Nonlinear Structural Problems

In this section, the design sensitivity expression for a response functional related to nonlinear problems in structural mechanics is derived. The stated principle and the incremental procedure for nonlinear analysis are used in the derivation. The reference domain approach is used; however, the material derivative procedure can also be derived just as for the linear problems. The design sensitivity expressions have been verified using several analytical examples[18,33] as well as numerical problems.[19,34]

A. Nonlinear Analysis

One major departure from linear analysis in nonlinear analysis is that quantities must be measured in a deformed configuration; in other words, undeformed and deformed configurations do not coincide in nonlinear analysis, and a reference configuration for the quantities must be defined. Because of the nature of the present paper, only the necessary equations are presented; additional details can be found in the literature.[11] Matrix and tensor notations and the total Lagrangian (TL) formulation are used, although the updated Lagrangian formulation can also be used. A left superscript indicates the configuration in which the quantity occurs, and a left subscript indicates the reference configuration. Also using the control volume concept of an earlier section, all equations are transformed to a reference domain.

Using the TL formulation, the equilibrium equation for the body at the time t (load level t) is given as

$$\int {}^t_0\boldsymbol{S}\cdot\delta^t_0\varepsilon J\, {}^r dV - \int {}^t_0\boldsymbol{f}\cdot\delta^t\boldsymbol{u}J\, {}^r dV - \int {}^t_0\boldsymbol{T}^0\cdot\delta^t\boldsymbol{u}J_s\, {}^r dS_T = 0 \tag{62}$$

where all of the quantities are referred to the initial or undeformed configuration, "·" refers to the standard tensor product, ${}^0V$ = undeformed volume of the body, ${}^t_0\boldsymbol{S}$ = second Piola-Kirchhoff stress tensor, ${}^t_0\varepsilon$ = Green-Lagrange strain tensor, ${}^t_0\boldsymbol{f}$ = body force per unit volume, ${}^t\boldsymbol{u}$ = displacement field, ${}^t_0\boldsymbol{T}^0$ = surface traction specified on part of the surface ${}^0S_T$, and δ = operator for arbitrary but kinematically admissible state fields.

The Green-Lagrange strain tensor and its arbitrary variation are given as

$$ {}^t_0\varepsilon = \tfrac{1}{2}[\overline{X}^T({}_r\nabla^t\boldsymbol{u}) + ({}_r\nabla^t\boldsymbol{u})^T\overline{X} + \overline{X}^T({}_r\nabla^t\boldsymbol{u})({}_r\nabla^t\boldsymbol{u})^T\overline{X}] \tag{63}$$

$$\delta^t_0\varepsilon = {}_0\boldsymbol{e}(\delta^t\boldsymbol{u}) \tag{64}$$

$${}_0\boldsymbol{e}(\ ) = \tfrac{1}{2}[\overline{X}^T({}_r\nabla(\ )) + ({}_r\nabla(\ ))\overline{X} + \overline{X}^T({}_r\nabla^t\boldsymbol{u})({}_r\nabla(\ ))^T\overline{X} + \overline{X}^T({}_r\nabla(\ ))({}_r\nabla^t\boldsymbol{u})^T\overline{X}] \tag{65}$$

where $\overline{X} = X^{-1}$, the subscript or superscript r refers to the coordinates in the reference domain, and ${}_r\nabla^t\boldsymbol{u} = [\partial^t u_i/\partial^r x_j]$. The nonlinear stress-strain law is written as

$${}^t_0\boldsymbol{S} = \phi({}^t_0\varepsilon,\boldsymbol{b}) \tag{66}$$

It is important to note that, for many applications, the functional form for ϕ is not known. In numerical implementations, the explicit form is not needed. Only an incremental stress-strain relation is required. History-dependent material models were also treated in Refs. 3 and 33 using the design sensitivity analysis principle.

In the incremental solution procedure, the strain at t is known and at $t + \Delta t$ it is decomposed as ${}^{t+\Delta t}_0\varepsilon = {}^t_0\varepsilon + {}_0\varepsilon$

with the increment $_0\varepsilon$ given as

$$_0\varepsilon = {}_0e(u) + \tfrac{1}{2}[\bar{X}^T({}_r\nabla u)({}_r\nabla u)^T\bar{X}] \quad (67)$$

where u is increment in the displacement field given as $u = {}^{t+\Delta t}u - {}^tu$. Since $\delta^{t+\Delta t}_0\varepsilon = \delta_0\varepsilon$, the virtual work principle at $t + \Delta t$ is written as

$$\int({}^t_0S + {}_0S)\cdot\delta_0\varepsilon J\,{}^r\mathrm{d}V - \int({}^{t+\Delta t}_0f\cdot\delta u)J\,{}^r\mathrm{d}V - \int({}^{t+\Delta t}_0T^0\cdot\delta u)J_s\,{}^r\mathrm{d}S_T = 0 \quad (68)$$

where $_0S$ is increment in the 2nd Piola-Kirchhoff stress and $\delta_0\varepsilon$ is given as

$$\delta_0\varepsilon = {}_0e(\delta u) + {}_0\eta(u,\delta u) \quad (69)$$

$${}_0\eta(u,\delta u) = \tfrac{1}{2}[\bar{X}^T({}_r\nabla u)({}_r\nabla u)^T\bar{X} + \bar{X}^T({}_r\nabla\delta u)({}_r\nabla u)^T\bar{X}] \quad (70)$$

Since Eq. (68) is still nonlinear, we linearize it by neglecting the term ${}_0S\cdot{}_0\eta(u,\delta u)$:

$$\int {}_0S\cdot{}_0e(\delta u)J\,{}^r\mathrm{d}V + \int {}^t_0S\cdot{}_0\eta(u,\delta u)J\,{}^r\mathrm{d}V - \int({}_0f\cdot\delta u)J\,{}^r\mathrm{d}V - \int({}_0T^0\cdot\delta u)J_s\,{}^r\mathrm{d}S_T = 0 \quad (71)$$

where $_0f$ and $_0T$ are increments in the body force and surface traction, respectively. This equation is obtained from Eq. (68) after eliminating the terms that correspond to the equilibrium equation at time t. The linearized constitutive law is given as

$${}_0S = \phi_{,\varepsilon}\cdot{}_0e(u) \quad (72)$$

B. Response Functional

The general response functional requiring sensitivity analysis is written in the reference domain as

$$\psi = \int G({}^t_0S,{}^t_0\varepsilon,{}^tu,b)J\,{}^r\mathrm{d}V + \int g({}^tu,{}^t_0T,b)J_s\,{}^r\mathrm{d}S_u + \int h({}^tu,{}^t_0T^0,b)J_s\,{}^r\mathrm{d}S_T \quad (73)$$

where S_u is that part of the surface S where the displacement is prescribed. This functional can be used to represent stress, strain, displacement, and reaction force constraints.

C. Design Sensitivity Analysis

To perform the design sensitivity analysis using the principle, replace the virtual state fields in the equilibrium equation (62) by the unknown adjoint fields and add it to the constraint functional of Eq. (73) to define the augmented functional of Eq. (4) as

$$L = \int(G - {}^t_0S\cdot\varepsilon^a + {}^t_0f\cdot u^a)J\,{}^r\mathrm{d}V + \int(g + {}^t_0T\cdot u^{a0})J_s\,{}^r\mathrm{d}S_u + \int(h + {}^t_0T^0\cdot u^a)J_s\,{}^r\mathrm{d}S_T \quad (74)$$

where the equilibrium equation (62) is written as

$$W^a \equiv \int(-{}^t_0S\cdot\varepsilon^a + {}^t_0f\cdot u^a)J\,{}^r\mathrm{d}V + \int {}^t_0T\cdot u^{a0}J_s\,{}^r\mathrm{d}S_u + \int {}^t_0T^t\cdot u^aJ_s\,{}^r\mathrm{d}S_T = 0 \quad (75)$$

Note that the integral over the displacement-specified boundary has been added to calculate the design sensitivity coefficient of the reaction force. Since ε^a has to be compatible with u^a, it is defined using the arbitrary variation of the Green-Lagrange strain tensor given in Eq. (64) as

$$\varepsilon^a = {}_0e(u^a) \quad (76)$$

Now Eq. (6) of the principle gives the total design variation of the constraint functional as $\bar{\delta}\psi = \bar{\bar{\delta}}L$, i.e.,

$$\bar{\delta}\psi = \int[(\bar{\bar{\delta}}G - \bar{\bar{\delta}}{}^t_0S\cdot\varepsilon^a - {}^t_0S\cdot\bar{\bar{\delta}}\varepsilon^a + \bar{\bar{\delta}}{}^t_0f\cdot u^a)J + (G - {}^t_0S\cdot\varepsilon^a + {}^t_0f\cdot u^a)\bar{\bar{\delta}}J]\,{}^r\mathrm{d}V + \int[(\bar{\bar{\delta}}g + \bar{\bar{\delta}}{}^t_0T\cdot u^{a0} + {}^t_0T\cdot\bar{\bar{\delta}}u^{a0})J_s + (g + {}^t_0T\cdot u^{a0})\bar{\bar{\delta}}J_s]\,{}^r\mathrm{d}S_u + \int[(\bar{\bar{\delta}}h + \bar{\bar{\delta}}{}^t_0T^0\cdot u^a)J_s + (h + {}^t_0T\cdot u^{a0})\bar{\bar{\delta}}J_s]\,{}^r\mathrm{d}S_T \quad (77)$$

According to Eq. (5), stationarity condition for L with respect to the state fields (i.e., $\tilde{\delta}L = 0$) gives

$$\int(\tilde{\delta}G - \tilde{\delta}{}^t_0S\cdot\varepsilon^a - {}^t_0S\cdot\tilde{\delta}\varepsilon^a + {}^t_0f\cdot\tilde{\delta}u^a)J\,{}^r\mathrm{d}V + \int(\tilde{\delta}g + \tilde{\delta}{}^t_0T\cdot u^{a0})J_s\,{}^r\mathrm{d}S_u + \int(\tilde{\delta}h + {}^t_0T^0\cdot\tilde{\delta}u^a)J_s\,{}^r\mathrm{d}S_T = 0 \quad (78)$$

Using Eq. (73), we get

$$\tilde{\delta}G = G_{,S}\cdot\tilde{\delta}{}^t_0S + G_{,\varepsilon}\cdot\tilde{\delta}{}^t_0\varepsilon + G_{,u}\cdot\tilde{\delta}{}^tu \quad (79)$$

$$\tilde{\delta}g = g_{,T}\cdot\tilde{\delta}{}^t_0T; \qquad \tilde{\delta}h = h_{,u}\cdot\tilde{\delta}{}^tu \quad (80)$$

Define the following quantities in Eqs. (79) and (80) for the adjoint structure:

$$\text{Initial strain field: } \varepsilon^{aI} = G_{,S} \text{ in } V \quad (81)$$

$$\text{Initial stress field: } S^{aI} = G_{,\varepsilon} \text{ in } V \quad (82)$$

$$\text{Body force: } f^a = G_{,u} \text{ in } V \quad (83)$$

$$\text{Specified Displacement: } u^{a0} = -g_{,T} \text{ on } S_u \quad (84)$$

$$\text{Specified Traction: } T^{a0} = h_{,u} \text{ on } S_T \quad (85)$$

Substituting Eqs (79–85) into Eq. (78) and collecting terms, we get

$$\int[-(\varepsilon^a - \varepsilon^{aI})\cdot\tilde{\delta}{}^t_0S + S^{aI}\cdot\tilde{\delta}{}^t_0\varepsilon + f^a\cdot\tilde{\delta}{}^tu - {}^t_0S\cdot\tilde{\delta}\varepsilon^a + {}^t_0f\cdot\tilde{\delta}u^a]J\,{}^r\mathrm{d}V + \int(-u^{a0}\cdot\tilde{\delta}{}^t_0T + \tilde{\delta}{}^t_0T\cdot u^{a0})J_s\,{}^r\mathrm{d}S_u + \int(T^{a0}\cdot\tilde{\delta}{}^tu + {}^t_0T^0\cdot\tilde{\delta}u^a)J_s\,{}^r\mathrm{d}S_T = 0 \quad (86)$$

Design variation of the constitutive law in Eq. (66) gives

$$\tilde{\delta}{}^t_0S = \phi_{,\varepsilon}\cdot{}_0e(\tilde{\delta}{}^tu); \qquad \tilde{\delta}{}^t_0\varepsilon = {}_0e(\tilde{\delta}{}^tu) \quad (87)$$

Substituting Eq. (87) into Eq. (86) and collecting terms, we get

$$\int[-\{(\varepsilon^a - \varepsilon^{aI})\cdot\phi_{,\varepsilon} - S^{aI}\}\cdot{}_0e(\tilde{\delta}{}^tu) + f^a\cdot\tilde{\delta}{}^tu - {}^t_0S\cdot\tilde{\delta}\varepsilon^a + {}^t_0f\cdot\tilde{\delta}u^a]J\,{}^r\mathrm{d}V + \int(T^{a0}\cdot\tilde{\delta}{}^tu + {}^t_0T^0\cdot\tilde{\delta}u^a)J_s\,{}^r\mathrm{d}S_T = 0 \quad (88)$$

Let the stress-strain law for the adjoint structure be defined as

$$S^a = \phi_{,\varepsilon}^{\,T}\cdot(\varepsilon^a - \varepsilon^{aI}) - S^{aI} \tag{89}$$

Thus, Eq. (88) can be rearranged as

$$\left\{\int(-S^a\cdot{}_0e(\bar{\delta}^t u) + f^a\cdot\bar{\delta}^t u)J\,{}^r\mathrm{d}V + \int T^{a0}\cdot\bar{\delta}^t u J_s\,{}^r\mathrm{d}S_T\right\}$$
$$+ \left\{\int(-{}^t_0S\cdot\bar{\delta}\varepsilon^a + {}^t_0f\cdot\bar{\delta}u^a)J\,{}^r\mathrm{d}V + \int {}^t_0T^0\cdot\bar{\delta}u^a J_s\,{}^r\mathrm{d}S_T\right\} = 0 \tag{90}$$

Note that the terms in the second pair of braces will represent the equilibrium equation for the primary structure if $\bar{\delta}\varepsilon^a$ is compatible with $\bar{\delta}u^a$. Arbitrary variation of the adjoint strain in Eq. (76) gives

$$\bar{\delta}\varepsilon^a = {}_0e(\bar{\delta}u^a) + {}_0\eta(u^a,\bar{\delta}^t u) \tag{91}$$

It can be observed from Eq. (91) that $\bar{\delta}\varepsilon^a$ is not compatible with $\bar{\delta}u^a$; however, ${}_0e(\bar{\delta}u^a)$ is compatible with $\bar{\delta}u^a$. Therefore, the equilibrium equation for the primary structure can be written as

$$\int(-{}^t_0S\cdot{}_0e(\bar{\delta}u^a) + {}^t_0f\cdot\bar{\delta}u^a)J\,{}^r\mathrm{d}V$$
$$+ \int {}^t_0T\cdot\bar{\delta}u^a J_s\,{}^r\mathrm{d}S_T = 0 \tag{92}$$

Substituting Eq. (92) into Eq. (90), we get

$$\int S^a\cdot{}_0e(\bar{\delta}^t u)J\,{}^r\mathrm{d}V + \int {}^t_0S\cdot{}_0\eta(u^a,\bar{\delta}^t u)J\,{}^r\mathrm{d}V$$
$$- \int f^a\cdot\bar{\delta}^t u J\,{}^r\mathrm{d}V - \int T^a{}_0\cdot\bar{\delta}^t u J_s\,{}^r\mathrm{d}S_T = 0 \tag{93}$$

This is then the equilibrium equation for the adjoint structure. Comparing the adjoint equation (93) with the incremental equilibrium equation (71) for the primary structure at the final load level t, it is clear that the stiffness of the adjoint structure is the tangent stiffness of the primary structure at the final load level. The adjoint equation is linear, but it depends on the state fields of the primary structure for the nonlinear case.

The design sensitivity formula given in Eq. (77) is the same as derived in Ref. 18. To compute the design sensitivity coefficients, one must solve the adjoint equation (92) with the initial conditions given in Eqs. (81–85), the adjoint strain-displacement equation (76), and the adjoint stress-strain law given in Eq. (87).

VI. Dynamic Problems

As for the structural problems, both continuum and discrete dynamic models can be treated with the principle. Only discrete models are discussed here; however, dynamic systems modeled with the continuum formulation have also been treated recently.[15,35]

Consider dynamic systems governed by the equation of motion written in the first-order form as

$$P(b)\dot{z} = f(b,z,t), \qquad 0 \le t \le T \tag{94}$$

with the initial conditions as $z(0) = z^0$. Here P is an $n \times n$ matrix that depends on the design variable vector $b \in R^k$, and $z(t)$ is an n-dimensional state variable vector. Equation (94) can be used to model linear and nonlinear, damped or undamped systems. The problem of design sensitivity analysis is to determine the gradient of a dynamic response functional written in the integral form as

$$\psi = \int_0^T h(b,z,t)\,\mathrm{d}t \tag{95}$$

Different types of time-dependent constraints can be transformed to this integral form.[21,36]

To obtain the design sensitivity expression using the principle, define the augmented functional of Eq. (4) as

$$L = \int_0^T h(b,z,t)\,\mathrm{d}t + \int z^{aT}(P(b)\dot{z} - f(b,z,t))\,\mathrm{d}t$$
$$= \int[h + z^{aT}(P\dot{z} - f)]\,\mathrm{d}t = \int \bar{h}\,\mathrm{d}t \tag{96}$$

where

$$\bar{h} = h + z^{aT}(P\dot{z} - f)$$

where the second integral in Eq. (96) is identified as the weak form of the governing equation $W^a = 0$, and $z^a(t)$ is an adjoint variable vector that needs to be determined. With use of the principle [i.e., Eq. (6)], the design sensitivity expression is given as

$$\bar{\delta}\psi = \bar{\bar{\delta}}L = \int \bar{h}_{,b}\cdot\delta b\,\mathrm{d}t$$
$$= \int_0^T [h_{,b} + ((P\dot{z} - f)_{,b})^T z^a]\cdot\delta b\,\mathrm{d}t \tag{97}$$

which is the same as given in Refs. 21 and 36.

To define the adjoint problem, we use Eq. (5) as

$$\bar{\delta}L = \int(\bar{h}_{,z}\cdot\bar{\delta}z + \bar{h}_{,\dot{z}}\cdot\bar{\delta}\dot{z})\,\mathrm{d}t = 0$$

Integrating by parts,

$$\int\left(\bar{h}_{,z} - \frac{\mathrm{d}}{\mathrm{d}t}(\bar{h}_{,\dot{z}})\right)\cdot\bar{\delta}z\,\mathrm{d}t + \bar{h}_{,\dot{z}}\cdot\bar{\delta}z\Big|_0^T = 0$$

Since $\bar{\delta}z(t)$ is arbitrary and $\bar{\delta}z(0) = \mathbf{0}$, we get the Euler-Lagrange equation:

$$\bar{h}_{,z} - \frac{\mathrm{d}}{\mathrm{d}t}(\bar{h}_{,\dot{z}}) = 0 \quad \text{with} \quad \bar{h}_{,\dot{z}}(T) = 0 \tag{98}$$

Substituting for $\bar{h}$ from Eq. (96) into Eq. 98),

$$P^T\dot{z}^a + f_{,z}^{\,T}z^a = h_{,z} \quad \text{with} \quad z^a(T) = 0 \tag{99}$$

Equation (99) defines the terminal value problem for the adjoint variables $z^a(t)$.

In dynamics of structures, usually the second-order form for the equations of motion is used:

$$M\ddot{z} + C\dot{z} + Kz = R \tag{100}$$

with initial conditions as $z(0) = \dot{z}(0) = \mathbf{0}$ and R as the equivalent load vector. The design sensitivity analysis principle can also be used with this form of the state equation. The Euler-Lagrange equation (98) in this case becomes

$$\bar{h}_{,z} - \frac{\mathrm{d}}{\mathrm{d}t}(\bar{h}_{,\dot{z}}) + \frac{\mathrm{d}^2}{\mathrm{d}t^2}(\bar{h}_{,\ddot{z}}) = \mathbf{0} \tag{101}$$

with the terminal conditions as

$$\bar{h}_{,\dot{z}}(T) = \mathbf{0} \quad \text{and} \quad \bar{h}_{,z}(T) - \frac{\mathrm{d}}{\mathrm{d}t}\bar{h}_{,\ddot{z}}(T) = \mathbf{0} \qquad (102)$$

In this case $\bar{h}$ is given as

$$\bar{h} = h + z^{aT}(M\ddot{z} + C\dot{z} + Kz - R) \qquad (103)$$

Thus, the Euler-Lagrange equation that determines the adjoint variable z^a is given from Eq. (101) as

$$M^T\ddot{z}^a - C^T\dot{z}^a + K^T z^a = -h_{,z}$$
$$\text{with} \quad z^a(T) = \mathbf{0}, \dot{z}^a(T) = \mathbf{0} \qquad (104)$$

This terminal value problem can be transformed to the initial value problem using the independent variable transformation.[21]

Equations (103) and (5) give the design sensitivity expression as

$$\delta\psi = \int_0^T \{h_{,b} + [(M\ddot{z} + C\dot{z} + Kz - R)_{,b}]^T z^a\}\cdot\delta b \, \mathrm{d}t \qquad (105)$$

VII. Discussion and Conclusions

A general variational principle for derivation of design sensitivity expressions for a wide variety of design problems is stated and proved without reference to a specific application. The principle is a generalization of the adjoint method of design sensitivity analysis that has been developed for various applications. Thus, it has unified a number of previous results. The principle is demonstrated on a few smooth linear and nonlinear problems. With proper mathematical care, it is also applicable to nonsmooth problems. The beauty of the principle is that it can be applied to discrete as well as continuum models, shape and nonshape design problems, and material derivative and reference domain/control volume formulations. The governing state equations may be given in the discretized matrix form, differential form, or variational form. The principle can be used with all of these forms. It is demonstrated on discrete as well as continuum models. Discretization of the continuum design sensitivity expressions, the analysis expressions, and the adjoint equations can be carried out using the standard Rayleigh-Ritz, Galerkin, or finite element methods.

The principle can also be used to derive design sensitivity expressions for static and dynamic response structural problems with general boundary conditions, similar to the ones derived in Refs. 37 and 38. It can be used to obtain the design sensitivity expressions when the structure is analyzed using substructures, as discussed in Ref. 39.

In conclusion, the design sensitivity analysis principle presented in this paper appears to be quite general. It seems to be applicable to other fields, such as linear and nonlinear heat transfer and fluid dynamic problems.

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