

Adjoint Sensitivity Analysis for Nonlinear Dynamic Thermoelastic Systems

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An adjoint approach is presented to formulate explicit sensitivities for a general functional associated with a nonlinear, dynamic, thermoelastic system. Uncoupled thermoelastic response and small-deformation behavior are assumed. The formulation uses the Lagrange multiplier method to define an adjoint system, the convolution operator to incorporate transient effects, and domain parameterization to describe shape variations. Variations of the functional are expressed in explicit form with respect to perturbations of the design fields: structural shape, material properties, applied loads, prescribed boundary conditions, and initial conditions. The functional is defined in terms of the design fields and the implicit response fields: displacement, temperature, strain, temperature gradient, stress, heat flux vector, reaction force, and reaction surface flux. In an example problem, the finite element method is used to evaluate the real and adjoint responses and the shape sensitivities for a tank design problem. The tank is modeled as a nonlinear, quasistatic, uncoupled, thermoelastic system.

I. Introduction

TECHNIQUES for explicit sensitivity analysis of thermal and mechanical systems have undergone rapid development in recent years. These formulations enable one to determine the response variation of a system with respect to perturbations of the design fields. This type of information is useful in optimal design algorithms,¹ identification problems,² reliability analyses,³ and inverse problems.⁴

The present development extends earlier work presented in the literature. Dems and Mroz⁵ derived explicit sensitivities using direct differentiation and an adjoint approach⁶ based on the reciprocity between a fictitious (adjoint) thermoelastic system and the variations of the real thermoelastic system. This small-displacement formulation includes a nonlinear, elastic stress-strain relationship. Meric⁷ presented design sensitivities for steady-state, linear, thermoelastic systems using an adjoint approach derived from the Lagrange multiplier method.⁸ Again, using the Lagrange multiplier method, Meric^{9,10} formulated shape sensitivities for steady-state, nonlinear, thermal systems. Shape sensitivities for linear elastic problems have been previously derived in Refs. 11–18. Some of these methods are applied to the thermoelastic problem in Refs. 5, 9, and 10, where explicit sensitivities for shape variations are derived using the boundary version of the material derivative method.¹⁴ Sensitivity analyses for transient problems are derived by adjoint methods in Refs. 14 and 18–22. The use of a time mapping¹⁴ in the adjoint problem is incorporated by Dems and Mroz⁵ to derive sensitivities of dynamic thermoelastic systems. Sensitivity formulations for additional nonlinear problems have also been presented; see Refs. 17 and 23–29 for nonlinear elastostatic derivations and Ref. 22 for a nonlinear transient conduction derivation.

Herein, the adjoint approach is utilized to formulate the sensitivities rather than the direct differentiation approach. In the adjoint method, the response fields from a second adjoint problem are determined and then used to directly evaluate the sensitivities. This technique requires the solution of two adjoint problems for each of the response functionals, regardless of the number of design parameters. In the direct differentiation approach, the partial derivatives of the response fields are determined with respect to each of the design parameters. The chain rule is then employed to evaluate the sensitivities. This latter technique requires the solution of two additional problems for each design parameter, regardless of the number of design functions. The choice of which technique to use depends on the information required, the ratio between the number of design functionals and design parameters, and the effort required to evaluate the sensitivity integrals.⁵

In the present work, the explicit sensitivities are derived for a generalized design functional describing the response of a nonlinear, dynamic, thermoelastic system. The design functional can be defined by any combination of the explicit design fields (material properties, applied loads, prescribed boundary conditions, initial conditions, and shape) and implicit response fields (displacement, temperature, strain, temperature gradient, stress, heat flux vector, reaction force, and reaction surface flux). Here, velocity, acceleration, and temperature rate are not considered. These response fields could be incorporated by using the methodology in Refs. 18 and 21.

The formulation utilizes an adjoint approach based on the Lagrange multiplier method. The conservation laws, constitutive models, strain-displacement relation, temperature-temperature gradient relation, and boundary conditions are adjoined to the response functional via the convolution operator. The Lagrange multipliers are equated to the response fields of fictitious elastodynamic and transient thermal systems (the adjoint problems). The convolution operator^{21,22,30} is incorporated in lieu of the time mappings required in other transient adjoint sensitivity derivations. Domain parameterization^{15–18,21,22} is used to describe shape variations.

This derivation accounts for nonlinearities in the stress, heat flux, and enthalpy constitutive relationships, and the descriptions of the internal heat source and applied surface flux distributions. Finite strains, large rotations, large temperature gradients, and history-dependent material properties are not

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considered. Deformation effects are neglected from the energy conservation law, and thus the formulation is only valid for uncoupled thermoelastic systems.

The formulation is presented in four sections. In the next section, the sensitivity problem is stated. Explicit sensitivities are derived separately in Secs. 3 and 4 for variations of the shape-independent and shape-dependent design fields. The equations are linearized for numerical implementation in Sec. 5. In Sec. 6, an example is presented in which the finite element method is used to evaluate the real and adjoint responses and the shape sensitivities of a tank design problem. The tank is modeled as a nonlinear, quasistatic, uncoupled, thermoelastic system.

II. Sensitivity Analysis Problem, δG

Consider the general functional that characterizes the performance of a nonlinear, dynamic, uncoupled, thermoelastic system. (Latin indices denote components with respect to a Cartesian coordinate system, and summation convention is used throughout this paper.)

$$G = \int_0^t \int_B f(u_i, \vartheta, E_{ij}, g_i, S_{ij}, q_i, e, \rho, b_i, r) dv + \int_{\partial B} g(u_i, s_i, \vartheta, q^s) da \quad (1)$$

The displacement $u(x, \tau)$, temperature $\vartheta(x, \tau)$, infinitesimal strain $E(x, \tau)$, temperature gradient $g(x, \tau)$, Cauchy stress $S(x, \tau)$, heat flux vector $q(x, \tau)$, surface traction $s(x, \tau)$, and surface flux $q^s(x, \tau)$ are all implicitly defined response fields. The heat supply $r(\vartheta, \phi)$ and internal energy $e(\vartheta, \phi)$ are modeled as functions of temperature and certain explicit design fields (e.g., material properties), which are collected in the design vector field $\phi(x, \tau)$. The ϕ consists of all the explicit design fields that are independent of shape. For example, the mass density $\rho(x)$ and body force $b(x, \tau)$ are explicitly defined design fields and are elements of ϕ . The τ represents the independent time variable, t is the terminal time in the analysis interval $(0, t)$, and x denotes the position vector. All field quantities are defined over the region B or its boundary ∂B with unit outward normal vector n . The fields are assumed to be smooth enough to justify the operations performed, and G is assumed to be differentiable with respect to its arguments. Note that is not always the case.¹⁴ For example, the response at a re-entrant cusp is not differentiable with respect to shape variations. Although G is expressed in integral form, it can be used to represent localized quantities in time and/or space by the incorporation of Dirac delta or local weighting functions. In Sec. 4, the shape of the structure is considered to be variable. In this case, all design fields are expressed as functions of a reference configuration, and x is also treated as a design field.

The response fields are implicitly determined by the design fields and the mixed boundary-initial-value problems for a dynamic uncoupled thermoelastic system³¹:

$$i^* S_{ij,j} + \beta_i = \rho u_i \quad \text{in } B \times [0, t] \quad (2)$$

$$S_{ij} = \hat{S}_{ij}(E, \vartheta, \phi) \quad \text{in } B \times [0, t] \quad (3)$$

$$E_{ij} = \frac{1}{2} (u_{i,j} + u_{j,i}) \quad \text{in } B \times [0, t] \quad (4)$$

$$s_i = S_{ij} n_j \quad \text{on } \partial B \times [0, t] \quad (5)$$

$$u_i = u_i^p \quad \text{on } A_u \times [0, t] \quad (6)$$

$$s_i = s_i^p \quad \text{on } A_s \times [0, t] \quad (7)$$

and

$$-1^* q_{i,i} + R = e \quad \text{in } B \times [0, t] \quad (8)$$

$$q_i = \hat{q}_i(\vartheta, g, \phi) \quad \text{in } B \times [0, t] \quad (9)$$

$$g_i = \vartheta_{,i} \quad \text{in } B \times [0, t] \quad (10)$$

$$q^s = q_i n_i \quad \text{on } \partial B \times [0, t] \quad (11)$$

$$\vartheta = \vartheta^p \quad \text{on } A_\vartheta \times [0, t] \quad (12)$$

$$q^s = q^p \quad \text{on } A_q \times [0, t] \quad (13)$$

In the above, $(\cdot)_{,i} \equiv \partial(\cdot)/\partial x_i$, and following the notation in Ref. 31, $*$ denotes the convolution operator, and $i \equiv \tau$. The nonlinear constitutive relations \hat{S} and \hat{q} are similar to e and q^s in that they are also functions of the implicit response and the design field vector. $\beta(x, \tau)$ and $R(r, e^0)$ are the psuedo body force and psuedoheat supply defined, by

$$\beta_i(x, \tau) = i^* b_i(x, \tau) + \rho(x) [u_i^0(x) + r v_i^0(x)] \quad (14)$$

$$R(r, e^0) = 1^* r(\vartheta, \phi) + e^0(\vartheta^0, \phi^0) \quad (15)$$

where $u^0(x)$ and $v^0(x)$ represent the initial displacement and velocity fields. The initial internal energy is $e^0 = e|_{\tau=0}$, which is dependent on the initial temperature field $\vartheta^0(x)$ and initial design vector field $\phi^0 = \phi|_{\tau=0}$. A_u and A_s are complementary subsurfaces of ∂B and correspond to surfaces with prescribed displacement $u^p(x, \tau)$ and prescribed traction $s^p(x, \tau)$. Similarly, the complementary subsurfaces A_ϑ and A_q have prescribed temperature $\vartheta^p(x, \tau)$ and prescribed flux $q^p(\vartheta, \phi)$. Since u^0 , v^0 , ϑ^0 , u^p , s^p , and ϑ^p are all explicitly defined, they are considered to be design fields and are included in ϕ . The function q^p is general enough to model radiation, nonlinear convection, or nonlinear heat flux boundary conditions.

In an effort to present the formulation in a concise manner, the design field is discretized. The design field vector is defined by a finite number of design parameters $\phi_\alpha, \alpha = 1, N$ and a suitable set of basis functions. For example, the density is expressed as $\rho'(x, \phi_\alpha)$. Here, the prime indicates that the function has been parameterized. Finite element models use this parameterization. In these models, material properties, applied loads, initial conditions, and boundary conditions are represented locally over each element by a number of discrete parameters and a set of interpolation functions defined over time and space.

The objective of this sensitivity derivation is to formulate an explicit expression for δG , in which only the variations of the design quantities are present; i.e., all reference to implicit response field variations are eliminated. In the next section, the design parameters ϕ_α are considered variable, the shape is held fixed, and the sensitivity δG_D is formulated. In the subsequent section, the design parameters are held fixed, the shape of the structure is varied, and the shape sensitivity δG_X is derived. The total functional variation δG is the sum $\delta G_D + \delta G_X$.

III. Variations of ϕ

In the present application of the Lagrange multiplier method, Eqs. (2–4), (6–10), and (12) and (13) are adjoined to

G via the convolution operator. The Lagrange multipliers, denoted by tildes, are equated to the response fields of an adjoint elastodynamic system and an adjoint transient thermal system. The augmented functional G^* is defined as

$$\begin{aligned}
 G^* = & \int_0^t \left[\int_B f(u_i, \vartheta, E_{ij}, g_i, S_{ij}, q_i, e', \rho', b_i', r') d\nu \right. \\
 & + \int_{\partial B} g(u_i, s_i, \vartheta, q^s) da \left. \right] d\tau + \frac{d^2}{d\tau^2} \left[\int_B \tilde{u}_i^* (i^* S_{ij,j} + \right. \\
 & + B_i' - \rho' u_i) d\nu \left. \right] + \frac{d}{d\tau} \left[\int_B \tilde{\vartheta}^* (-1^* q_{i,i} + R' - e') d\nu \right] \\
 & + \int_B \tilde{E}_{ij}^* (S_{ij} - \tilde{S}_{ij}') d\nu + \int_B \tilde{g}_i^* (\tilde{q}_i' - q_i) d\nu + \\
 & \int_B \tilde{S}_{ij}^* \left[E_{ij} - \frac{1}{2} (u_{i,j} + u_{j,i}) \right] d\nu + \int_B \tilde{q}_i^* (\vartheta_i - g_i) d\nu \\
 & + \int_{A_u} \tilde{s}_i^* (u_i - u_i') da + \int_{A_s} \tilde{u}_i^* (s_i' - s_i) da \\
 & + \int_{A_\vartheta} \tilde{q}^s (q^s - \vartheta) da + \int_{A_q} \tilde{\vartheta}^* (q^s - q^p) da \quad (16)
 \end{aligned}$$

The variation of G^* due to variations of ϕ_α , i.e., $\phi_\alpha \rightarrow \phi_\alpha + \delta\phi_\alpha$, is expressed (after an application of the divergence theorem) as

$$\begin{aligned}
 \delta G_D^* = & \left\{ \int_0^t \left[\int_B (f_{;e'} e'_{;\phi_\alpha} + f_{;\rho'} \rho'_{;\phi_\alpha} + f_{;b_i'} b_{i;\phi_\alpha} + \right. \right. \\
 & f_{;r'} r'_{;\phi_\alpha}) d\nu + \int_{A_u} g_{;u_i'} u_{i;\phi_\alpha}^p da + \\
 & \int_{A_s} g_{;s_i'} s_{i;\phi_\alpha}^p da + \int_{A_\vartheta} g_{;\vartheta'} \vartheta_{;\phi_\alpha}^p da + \\
 & \left. \int_{A_q} g_{;q^p'} q_{;\phi_\alpha}^p da \right] d\tau + \int_B \left[\frac{d^2}{d\tau^2} (\tilde{u}_i^* (B_{i;\phi_\alpha}' - \rho_{;\phi_\alpha}' u_i)) \right. \\
 & \left. + \frac{d}{d\tau} [\tilde{\vartheta}^* (R_{;\phi_\alpha}' - e_{;\phi_\alpha}')] - \tilde{E}_{ij}^* \tilde{S}_{ij;\phi_\alpha}' + \tilde{g}_i^* \tilde{q}_{i;\phi_\alpha}' d\nu - \right. \\
 & \int_{A_u} \tilde{s}_i^* u_{i;\phi_\alpha}' da + \int_{A_s} \tilde{u}_i^* s_{i;\phi_\alpha}' da + \int_{A_\vartheta} \tilde{q}^s s_{;\phi_\alpha}' da - \\
 & \left. \int_{A_q} \tilde{\vartheta}^* q_{;\phi_\alpha}' da \right] \delta\phi_\alpha + \int_B \left[1^* f_{;u_i} \delta u_i - \frac{d^2}{d\tau^2} (\tilde{u}_i^* \rho' \delta u_i) + \right. \\
 & \tilde{S}_{ij,i}^* \delta u_j \left. \right] d\nu - \int_{\partial B} \tilde{S}_{ij} n_j^* \delta u_i da + \int_B \left\{ 1^* (f_{;\vartheta} + f_{;r'} r'_{;\vartheta} + \right. \\
 & f_{;e'} e'_{;\vartheta}) \delta\vartheta + \frac{d}{d\tau} [\tilde{\vartheta}^* (R_{;\vartheta}' - e_{;\vartheta}')] - \tilde{E}_{ij}^* \tilde{S}_{ij;\vartheta}' + \tilde{g}_i^* \tilde{q}_{i;\vartheta}' \\
 & \left. - \tilde{q}_{i,i}^* \delta\vartheta - \tilde{q}_{i,i}^* \delta\vartheta \right\} d\nu + \int_{\partial B} \tilde{q}_i n_i^* \delta\vartheta da + \\
 & \int_B \left\{ 1^* f_{;S_{ij}} \delta S_{ij} - \frac{d^2}{d\tau^2} \left[\frac{1}{2} (\tilde{u}_{i,j} + \tilde{u}_{j,i})^* i^* \delta S_{ij} \right] + \right. \\
 & \tilde{E}_{ij}^* \delta S_{ij} \left. \right\} d\nu + \int_{\partial B} \frac{d^2}{d\tau^2} (\tilde{u}_i^* i^* \delta S_{ij}) n_j da + \\
 & \int_B \left[1^* f_{;q_i} \delta q_i + \frac{d}{d\tau} (\tilde{\vartheta}_{;i}^* 1^* \delta q_i) - \tilde{g}_i^* \delta q_i \right] d\nu - \\
 & \int_{\partial B} \frac{d}{d\tau} (\tilde{\vartheta}^* 1^* \delta q_i) n_i da + \int_B (1^* f_{;E_{kl}} \delta E_{kl} -
 \end{aligned}$$

$$\begin{aligned}
 & \tilde{E}_{ij}^* \tilde{S}_{ij;E_{kl}}' \delta E_{kl} + \tilde{S}_{kl}^* \delta E_{kl}) d\nu + \int_B (1^* f_{;g_j} \delta g_j + \\
 & \tilde{g}_i^* \tilde{q}_{i;g_j}' \delta g_j - \tilde{q}_j^* \delta g_j) d\nu + \int_{A_u} (1^* g_{;s_i} \delta s_i + \\
 & \tilde{s}_i^* \delta u_i) da + \int_{A_s} (1^* g_{;u_i} \delta u_i - \tilde{u}_i^* \delta s_i) da + \\
 & \int_{A_\vartheta} (1^* g_{;q^s} \delta q^s - \tilde{q}^s \delta\vartheta) da + \int_{A_q} \left[1^* (g_{;\vartheta} \delta\vartheta + \right. \\
 & g_{;q^p} q_{;\vartheta}' \delta\vartheta) + \tilde{\vartheta}^* (\delta q^s - q_{;\vartheta}' \delta\vartheta) \left. \right] da \quad (17)
 \end{aligned}$$

where $a_{;b} \equiv \partial a / \partial b$. In the above equation, the implicit response variations (δu , $\delta\vartheta$, δE , δg , δS , δq , δs , and δq^s) are constrained by the requirement that Eqs. (2-13) must be satisfied for the varied design $\phi_\alpha + \delta\phi_\alpha$. The objective here is to eliminate all direct reference to these response variations from the sensitivity expression.

Time differentiation, some rearranging of Eq. (17), and repeated use of the identity $d/d\tau (a^*b) = da/d\tau^*b + a|_{\tau=0^0}$ gives

$$\begin{aligned}
 \delta G_D^* = & \left\{ \int_0^t \left[\int_B (f_{;e'} e'_{;\phi_\alpha} + f_{;\rho'} \rho'_{;\phi_\alpha} + f_{;b_i'} b_{i;\phi_\alpha} + \right. \right. \\
 & f_{;r'} r'_{;\phi_\alpha}) d\nu + \int_{A_u} g_{;u_i'} u_{i;\phi_\alpha}^p da + \int_{A_s} g_{;s_i'} s_{i;\phi_\alpha}^p da + \\
 & \int_{A_\vartheta} g_{;\vartheta'} \vartheta_{;\phi_\alpha}^p da + \int_{A_q} g_{;q^p'} q_{;\phi_\alpha}^p da \left. \right] d\tau \\
 & + \int_B \left[\tilde{u}_i^* (b_{i;\phi_\alpha}' - \rho_{;\phi_\alpha}' \tilde{u}_i) + \right. \\
 & \tilde{u}_i(x, t) \rho' u_{i;\phi_\alpha}^{0'} + \tilde{u}_i(x, t) \rho' v_{i;\phi_\alpha}^{0'} + \tilde{\vartheta}^* (r_{;\phi_\alpha}' - \\
 & e'_{;\phi_\alpha}) + \tilde{\vartheta}(x, t) e_{;\vartheta}^{0'} \vartheta_{;\phi_\alpha}^{0'} - \tilde{E}_{ij}^* \tilde{S}_{ij;\phi_\alpha}' + \tilde{g}_i^* \tilde{q}_{i;\phi_\alpha}' \left. \right] d\nu - \\
 & \int_{A_u} \tilde{s}_i^* u_{i;\phi_\alpha}' da + \int_{A_s} \tilde{u}_i^* s_{i;\phi_\alpha}' da + \int_{A_\vartheta} \tilde{q}^s s_{;\phi_\alpha}' da - \\
 & \int_{A_q} \tilde{\vartheta}^* q_{;\phi_\alpha}' da \left. \right\} \delta\phi_\alpha + \int_B \left[1^* f_{;u_i} \delta u_i - \tilde{u}_i^* \rho' \delta u_i - \right. \\
 & \tilde{u}_i^0 \rho' \delta u_i(x, t) - \tilde{u}_i^0 \rho' \delta v_i(x, t) + \tilde{S}_{ij,i}^* \delta u_j \left. \right] d\nu + \\
 & \int_B \left[1^* (f_{;\vartheta} + f_{;r'} r'_{;\vartheta} + f_{;e'} e'_{;\vartheta}) \delta\vartheta + \tilde{\vartheta}^* r_{;\vartheta}' \delta\vartheta - \tilde{\vartheta}^* e_{;\vartheta}' \delta\vartheta - \right. \\
 & \tilde{\vartheta}^0 e_{;\vartheta,x,t}' \delta\vartheta(x, t) - \tilde{E}_{ij}^* \tilde{S}_{ij;\vartheta}' \delta\vartheta + \tilde{g}_i^* \tilde{q}_{i;\vartheta}' \delta\vartheta - \tilde{q}_{i,i}^* \delta\vartheta \left. \right] d\nu \\
 & + \int_B \left[1^* f_{;S_{ij}} \delta S_{ij} - \frac{1}{2} (\tilde{u}_{i,j} + \tilde{u}_{j,i})^* \delta S_{ij} + \tilde{E}_{ij}^* \delta S_{ij} \right] d\nu \\
 & + \int_B (1^* f_{;q_i} \delta q_i + \tilde{\vartheta}_{;i}^* \delta q_i - \tilde{g}_i^* \delta q_i) d\nu + \\
 & \int_B (1^* f_{;E_{kl}} \delta E_{kl} - \tilde{E}_{ij}^* \tilde{S}_{ij;E_{kl}}' \delta E_{kl} + \tilde{S}_{kl}^* \delta E_{kl}) d\nu + \\
 & \int_B (1^* f_{;g_j} \delta g_j + \tilde{g}_i^* \tilde{q}_{i;g_j}' \delta g_j - \tilde{q}_j^* \delta g_j) d\nu + \\
 & \int_{A_u} (1^* g_{;s_i} \delta s_i - \tilde{u}_i^* \delta S_{ij} n_j + \tilde{s}_i^* \delta u_i - \tilde{S}_{ij} n_j^* \delta u_i) da +
 \end{aligned}$$

$$\begin{aligned}
& \int_{A_s} (1^* g_{,u_i} \delta u_i + \tilde{S}_{ij} n_j^* \delta u_i - \tilde{u}_i^* S_{s_i} + \tilde{u}_i^* \delta S_{ij} n_j) da + \\
& \int_{A_\theta} (1^* g_{,q_s} \delta q^s - \tilde{\vartheta}^* \delta q_i n_i - \tilde{q}^s \delta \vartheta + \tilde{q}_i n_i^* \delta \vartheta) da + \\
& \int_{A_q} \left[1^* (g_{,p} \delta \vartheta + g_{,q p} q_{,p}^* \delta \vartheta) + \tilde{q}_i n_i^* \delta \vartheta - \tilde{\vartheta}^* \delta q_i n_i + \right. \\
& \left. \tilde{\vartheta}^* (\delta q^s - q_{,p}^* \delta \vartheta) \right] da \quad (18)
\end{aligned}$$

where $(\cdot) \equiv \frac{d(\cdot)}{d\tau}$; and $(\ddot{\cdot}) \equiv \frac{d^2(\cdot)}{d\tau^2}$.

To eliminate the integrands that contain response variations, two adjoint initial-boundary-value problems are defined and solved. The data for these problems are given by

$$\tilde{b}_i(x, t - \tau) = f_{,u_i} |_{(x,\tau)} \quad \text{in } B \times [0, t] \quad (19)$$

$$\tilde{E}_{ij}^A(x, t - \tau) = f_{,S_{ij}} |_{(x,\tau)} \quad \text{in } B \times [0, t] \quad (20)$$

$$\tilde{S}_{ij}^A(x, t - \tau) = -f_{,E_{ij}} |_{(x,\tau)} \quad \text{in } B \times [0, t] \quad (21)$$

$$\tilde{u}_i^p(x, t - \tau) = -g_{,s_i} |_{(x,\tau)} \quad \text{on } A_u \times [0, t] \quad (22)$$

$$\tilde{s}_i^p(x, t - \tau) = g_{,u_i} |_{(x,\tau)} \quad \text{on } A_s \times [0, t] \quad (23)$$

$$\tilde{u}_i^0(x) = 0 \quad \text{in } B \quad (24)$$

$$\tilde{v}_i^0(x) = 0 \quad \text{in } B \quad (25)$$

for the adjoint elastodynamic system and

$$\tilde{r}(x, t - \tau) = f_{,r} |_{(x,\tau)} + f_{,r'} |_{(x,\tau)} r'_{,i} |_{(x,\tau)} + f_{,e'} |_{(x,\tau)} e'_{,i} |_{(x,\tau)} - \tilde{E}_{ij}(x, t - \tau) \tilde{S}'_{ij,i} |_{(x,\tau)} \quad \text{in } B \times [0, t] \quad (26)$$

$$\tilde{g}_i^A(x, t - \tau) = -f_{,q_i} |_{(x,\tau)} \quad \text{in } B \times [0, t] \quad (27)$$

$$\tilde{q}_i^A(x, t - \tau) = f_{,g_j} |_{(x,\tau)} \quad \text{in } B \times [0, t] \quad (28)$$

$$\tilde{\vartheta}^p(x, t - \tau) = g_{,q^s} |_{(x,\tau)} \quad \text{on } A_\theta \times [0, t] \quad (29)$$

$$\tilde{q}^p(x, t - \tau) = -g_{,p} |_{(x,\tau)} - g_{,q p} |_{(x,\tau)} q_{,p}^* |_{(x,\tau)} + \tilde{\vartheta}(x, t - \tau) q_{,p}^* |_{(x,\tau)} \quad A_q \times [0, t] \quad (30)$$

$$\tilde{\vartheta}^0(x) = 0 \quad \text{in } B \quad (31)$$

for the adjoint transient thermal system. In the above, the applied terms (\tilde{E}^A , \tilde{S}^A , \tilde{g}^A , and \tilde{q}^A) are analogous to initial strain and stress tensors in elastic systems. However, these applied terms are time-dependent and not necessarily symmetric. This sort of adjoint data definition first appeared in Ref. 6.

The governing equations for the adjoint elastodynamic system are

$$\tilde{S}_{ij,j} + \tilde{b}_i = \rho' \ddot{\tilde{u}}_i \quad \text{in } B \times [0, t] \quad (32)$$

$$\tilde{E}_{ij} = \frac{1}{2} (\tilde{u}_{i,j} + \tilde{u}_{j,i}) - \tilde{E}_{ij}^A \quad \text{in } B \times [0, t] \quad (33)$$

$$\tilde{S}_{kl}(x, t - \tau) = \tilde{E}_{ij}(x, t - \tau) \tilde{S}'_{ij;E_{kl}} |_{(x,\tau)} + \tilde{S}_{kl}^A(x, t - \tau) \quad \text{in } B \times [0, t] \quad (34)$$

$$\tilde{s}_i = \tilde{S}_{ij} n_j \quad \text{in } \partial B \times [0, t] \quad (35)$$

For the adjoint transient thermal system they are

$$-\tilde{q}_{i,i}(x, t - \tau) + \tilde{\vartheta}(x, t - \tau) r'_{,i} |_{(x,\tau)} + \tilde{g}_i(x, t - \tau) \tilde{q}'_{i;\vartheta} |_{(x,\tau)} + \tilde{r}(x, t - \tau) = \tilde{\vartheta}(x, t - \tau) e'_{,i} |_{(x,\tau)} \quad \text{in } B \times [0, t] \quad (36)$$

$$\tilde{g}_i = \tilde{\vartheta}_{,i} - \tilde{g}_i^A \quad \text{in } B \times [0, t] \quad (37)$$

$$\tilde{q}_j(x, t - \tau) = \tilde{g}_i(x, t - \tau) \tilde{q}'_{i;g_j} |_{(x,\tau)} + \tilde{q}_j^A(x, t - \tau) \quad \text{in } B \times [0, t] \quad (38)$$

$$\tilde{q}^s = \tilde{q}_i n_i \quad \text{in } \partial B \times [0, t] \quad (39)$$

Two points should be noted in the above equations. First, the inclusion of $\tilde{E}(x, t - \tau) \tilde{S}' |_{(x,\tau)}$ in the definition of \tilde{r} necessitates the evaluation of the adjoint elastic response prior to the adjoint thermal response. Second, as noted in Refs. 5, 17, 22-29, and 32, the adjoint problems are linear. Thus, the adjoint systems generally require less effort to analyze than the real systems.

In finite element implementations, the Newton-Raphson iteration method is often used to evaluate the real response. In these formulations, the tangent stiffness matrices defined by the real elastic and real thermal systems at time τ are the transposes of those required to determine the adjoint elastic and thermal responses at time $t - \tau$. So once the real response is known, the adjoint response can be obtained in an efficient manner. When a reasonably tight convergence tolerance is used during the real analysis and sufficient storage is available, then the decomposed stiffness matrices from the real analysis at time τ can be stored and later utilized to determine the adjoint response at time $t - \tau$. This procedure requires no additional stiffness matrix assemblies or decompositions for the adjoint problem; only load vector assemblies and back substitutions are required to obtain the adjoint solution. Thus, the computational requirements for the adjoint analysis are much less than those for the real analysis which generally requires several iterations to converge at each time step.¹⁷ The tangent stiffness matrices might be nonsymmetric in a full Newton-Raphson formulation of the thermoelastic problem. However, if a hyperelastic constitutive model is used for the stress-strain relationship, then the elastic tangent stiffness matrix will be symmetric³³; and if the conductivity tensor [see Eq. (61)] is temperature-independent, then the thermal tangent stiffness matrix will be symmetric.³⁴ Transients are treated in the usual manner (e.g., Nemark-Beta and implicit time integration schemes³⁵).

Satisfaction of Eqs. (19-39) (i.e., the solution of the two adjoint problems) eliminates all of the integrals in Eq. (18) which contain the response variations. Then, $\delta G^* = \delta G^8$ and the explicit sensitivity are expressed as

$$\begin{aligned}
\delta G_D = & \left\{ \int_0^t \left[\int_B (f_{,e'} e'_{,\alpha} + f_{,p} p'_{,\alpha} + f_{,b_i} b'_{i,\alpha} + \right. \right. \\
& f_{,r} r'_{,\alpha}) dv + \int_{A_u} g_{,u p'} u'_{p;\phi_\alpha} da + \int_{A_s} g_{,s p'} s'_{p;\phi_\alpha} da \\
& + \int_{A_\theta} g_{,\vartheta p'} \vartheta'_{p;\phi_\alpha} da + \int_{A_q} g_{,q p'} q'_{p;\phi_\alpha} da \Big] d\tau + \\
& \int_B \left[\tilde{u}_i^* (b'_{i;\phi_\alpha} - \rho'_{,\phi_\alpha} \tilde{u}_i) + \tilde{u}_i(x, t) \rho' u'_{i;\phi_\alpha} + \right. \\
& \tilde{u}_i(x, t) \rho' v'_{i;\phi_\alpha} + \tilde{\vartheta}^* (r'_{,\phi_\alpha} - \dot{e}'_{,\phi_\alpha}) + \tilde{\vartheta}(x, t) e'_{,\phi_\alpha} - \\
& \tilde{E}_{ij}^* \tilde{S}'_{ij;\phi_\alpha} + \tilde{g}_i^* \tilde{q}'_{i;\phi_\alpha} \Big] dv - \int_{A_u} \tilde{s}_i^* u'_{i;\phi_\alpha} da + \\
& \int_{A_s} \tilde{u}_i^* s'_{i;\phi_\alpha} da + \int_{A_\theta} \tilde{q}^s s'_{,\phi_\alpha} da - \\
& \left. \int_{A_q} \tilde{\vartheta}^* q'_{,\phi_\alpha} da \right\} \delta \phi_\alpha \quad (40)
\end{aligned}$$

If either the thermal or elastic variables are omitted from this analysis, then the sensitivity formulation is valid for nonlinear elastodynamic and nonlinear transient conduction systems, respectively.

These results are consistent with those appearing in Ref. 5. In the present formulation, nonlinear thermal systems are treated, and adjoint time mappings are automatically incorporated by the convolution. Note that the convolution is employed as a formulation device; it has no effect on the numerical implementation relative to other methods, e.g., Refs. 14 and 19–22. When specialized for pure thermal systems, this formulation extends that presented in Ref. 9 for nonlinear steady-state conduction problems by incorporating transient behavior. These results are also consistent with those obtained in Refs. 17 and 24–29 for nonlinear elastostatic systems, although only small-deformation problems are considered here. The results agree with those appearing in Refs. 18, 21, and 22 for elastodynamic systems and linear and nonlinear transient thermal systems, respectively.

The adjoint governing equations are derived in this formulation using the Lagrange multiplier method. The formulations in Refs. 5, 16–18, and 21 state the adjoint governing equations a priori. In nonlinear problems, the correct adjoint governing equations might not be readily apparent.

IV. Shape Variations

In the domain parameterization method,^{11,12,15–18,21,22} a reference configuration B' with position vector r is introduced, and a deformation-like mapping is defined

$$x(r): B' \rightarrow B \quad (41)$$

In this way, the configuration B is defined by the image $x(B')$ and the variants of this configuration by $x(B') + \delta x(B')$.

G is written in terms of the reference geometry as

$$G = \int_0^t \left[\int_{B'} f(u_i, \vartheta, E_{ij}, g_{ij}, S_{ij}, q_i, e, \rho, b_i, r) J \, dv' + \int_{\partial B'} g(u_i, \vartheta, s_i, q^s) K \, da' \right] d\tau \quad (42)$$

where $J = dv'/dv$ is the determinant of the Jacobian tensor, $J_{ij} = x_{i,j}$; $(\cdot)_{,j} \equiv \partial(\cdot)/\partial x_j$; and $K = da'/da$ is a surface area metric.^{14,18} (Henceforth, the superscript $'$ denotes the appropriate body or surface quantity in the reference domain whose image under x corresponds to a body or surface quantity in the real domain. For example, dv' is the differential volume in B' that maps to dv in B .) In the above, all fields are expressed on B' , for example, $\phi = \phi(r, \tau)$.

Equations (2–13) are also transformed to the reference domain (see Refs. 18, 22, and 36), viz:

$$i^*(JJ_{jm}^{-1} S_{mi})_{,j} + B_i J = \rho u_i J \quad \text{in } B' \times [0, t] \quad (43)$$

$$S_{ij} = \hat{S}_{ij}(E, \vartheta, \phi_\alpha) \quad \text{in } B' \times [0, t] \quad (44)$$

$$E_{ij} = \frac{1}{2} (u_{i,m} J_{mj}^{-1} + u_{j,m} J_{mi}^{-1}) \quad \text{in } B' \times [0, t] \quad (45)$$

$$s_i K = JJ_{jm}^{-1} S_{mi} n_j^r \quad \text{on } \partial B' \times [0, t] \quad (46)$$

$$u_i = u_i^p \quad \text{on } A_u^r \times [0, t] \quad (47)$$

$$s_i = s_i^p \quad \text{on } A_s^r \times [0, t] \quad (48)$$

$$-1^*(q_i JJ_{mi}^{-1})_{,m} + RJ = eJ \quad \text{in } B' \times [0, t] \quad (49)$$

$$q_i = \hat{q}_i(\vartheta, g, \phi_\alpha) \quad \text{in } B' \times [0, t] \quad (50)$$

$$g_i = \vartheta_{,m} J_{mi}^{-1} \quad \text{in } B' \times [0, t] \quad (51)$$

$$q^s K = q_i JJ_{mi}^{-1} n_m^r \quad \text{on } \partial B' \times [0, t] \quad (52)$$

$$\vartheta = \vartheta^p \quad \text{on } A_\vartheta^r \times [0, t] \quad (53)$$

$$q^s = q^p \quad \text{on } A_q^r \times [0, t] \quad (54)$$

where J^{-1} is the inverse of the Jacobian tensor.

Equations (43–45), (47–51), and (53–54) are adjoined to G to define the augmented functional.

$$\begin{aligned} G^* = & \int_0^t \left[\int_{B'} f(u_i, \vartheta, E_{ij}, g_{ij}, S_{ij}, q_i, e, \rho, b_i, r) J \, dv' + \right. \\ & \left. \int_{\partial B'} g(u_i, s_i, \vartheta, q^s) K \, da' \right] d\tau + \frac{d^2}{d\tau^2} \left\{ \int_{B'} \tilde{u}_i^* \left[i^*(JJ_{jm}^{-1} S_{mi})_{,j} \right. \right. \\ & \left. \left. + B_i J - \rho u_i J \right] dv' \right\} + \frac{d}{d\tau} \left\{ \int_{B'} \tilde{\vartheta}^* \left[-1^*(q_i JJ_{mi}^{-1})_{,m} + \right. \right. \\ & \left. \left. RJ - eJ \right] dv' \right\} + \int_{B'} \tilde{E}_{ij}^* (S_{ij} - \hat{S}_{ij}) J \, dv' + \int_{B'} \tilde{g}_i^* \\ & \times (\hat{q}_i - q_i) J \, dv' + \int_{B'} \tilde{S}_{ij}^* \left[E_{ij} - \frac{1}{2} (u_{i,m} J_{mj}^{-1} + u_{j,m} J_{mi}^{-1}) \right] \\ & J \, dv' + \int_{B'} \tilde{q}_i^* (\vartheta_{,m} J_{mi}^{-1} - g_i) J \, dv' + \\ & \int_{A_u} \tilde{s}_i^* (u_i - u_i^p) K \, da' + \int_{A_s} \tilde{u}_i^* (s_i^p - s_i) K \, da' + \\ & \int_{A_\vartheta} \tilde{q}^{s*} (\vartheta^p - \vartheta) K \, da' + \int_{A_q} \tilde{\vartheta}^* (q^s - q^p) K \, da' \quad (55) \end{aligned}$$

In a manner analogous to the last section, the field $x(r)$ is parameterized by $x = x'(r, \varphi_\alpha)$, $\alpha = 1, M$. This technique is used in the isoparametric finite element method, where node coordinates are used with the element shape functions to locally define the mapping x' on the parent element. In this case, the node coordinates comprise the elements φ_α .

A variation of only φ_α and an application of the divergence theorem to G^* gives

$$\begin{aligned} \delta G^*_{\varphi_\alpha} = & \left\{ \int_0^t \left[\int_{B'} f(u_i, \vartheta, E_{ij}, g_{ij}, S_{ij}, q_i, e, \rho, b_i, r) J'_{,\varphi_\alpha} \, dv' + \right. \right. \\ & \left. \left. \int_{\partial B'} g(u_i, s_i, \vartheta, q^s) K'_{,\varphi_\alpha} \, da' \right] d\tau + \int_{B'} \left\{ \frac{d^2}{d\tau^2} \left[\tilde{u}_i^* (B_i - \right. \right. \right. \\ & \left. \left. \rho u_i) J'_{,\varphi_\alpha} \right] + \frac{d}{d\tau} \left[\tilde{\vartheta}^* (R - e) J'_{,\varphi_\alpha} \right] - \tilde{S}_{ij}^* u_{i,m} J'_{mj,\varphi_\alpha} J' + \right. \\ & \left. \left. \tilde{q}_i^* \vartheta_{,m} J'_{mi,\varphi_\alpha} J' \right\} dv' \right\} \delta \varphi_\alpha + \int_{B'} \left[1^* f_{,u_i} \delta u_i J' - \right. \\ & \left. \frac{d^2}{d\tau^2} (\tilde{u}_i^* \rho \delta u_i J') + (J' J'_{mj}^{-1})_{,m} \tilde{S}_{ij}^* \delta u_i \right] dv' - \\ & \int_{\partial B'} J' J'_{mj}^{-1} \tilde{S}_{ij} n_m^r \delta u_i \, da' + \int_{B'} \left\{ 1^* f_{,\vartheta} \delta \vartheta + \right. \\ & \left. f_{,e} e_{,\vartheta} J' \delta \vartheta + \frac{d}{d\tau} \left[\tilde{\vartheta}^* (R_{,\vartheta} - e_{,\vartheta}) J' \delta \vartheta \right] - \tilde{E}_{ij}^* + \tilde{S}_{ij,\vartheta} J' \delta \vartheta + \right. \\ & \left. \tilde{g}_i^* q_{i,\vartheta} J' \delta \vartheta - (\tilde{q}_i J' J'_{mi}^{-1})_{,m} \delta \vartheta \right\} dv' + \int_{\partial B'} \tilde{q}_i J' J'_{mi}^{-1} n_m^r \\ & \delta \vartheta \, da' + \int_{B'} \left\{ 1^* f_{,S_{mi}} \delta S_{mi} - \frac{d^2}{d\tau^2} \left[\frac{1}{2} (\tilde{u}_{i,j} J'_{jm}^{-1} + \right. \right. \\ & \left. \left. \tilde{u}_{m,j} J'_{ji}^{-1})^* i^* \delta S_{mi} \right] + \tilde{E}_{mi}^* \delta S_{mi} \right\} J' \, dv' + \end{aligned}$$

$$\begin{aligned}
& \int_{\partial B^r} \frac{d^2}{d\tau^2} (\tilde{u}_i^* i^* \delta S_{mi} J' J_{jm}^{-1} n_j^r) da^r - \int_{B^r} \frac{d^2}{d\tau^2} \\
& \times (\tilde{u}_{i,j} J_{jm;\varphi_\alpha}^{-1} J' i^* S_{mi} + \tilde{u}_{i,j} J_{jm}^{-1} J'_{;\varphi_\alpha} S_{mi}) \delta \varphi_\alpha d\nu^r + \\
& \int_{\partial B^r} \frac{d^2}{d\tau^2} (\tilde{u}_i^* i^* S_{mi} J' J_{jm;\varphi_\alpha}^{-1} n_m^r + \tilde{u}_i^* i^* S_{mi} J'_{;\varphi_\alpha} J_{jm}^{-1} n_m^r) \delta \varphi_\alpha \\
& \times da^r + \int_{B^r} \left[1^* f_{;q_i} \delta q_i + \frac{d}{d\tau} (\tilde{\vartheta}_{,m} J_{mi}^{-1} * 1^* \delta q_i) - \tilde{g}_i^* \delta q_i \right] J' \\
& \times d\nu^r - \int_{\partial B^r} \frac{d}{d\tau} (\tilde{\vartheta}^* 1^* \delta q_i J' J_{mi}^{-1} n_m^r) da^r + \\
& \int_{B^r} \frac{d}{d\tau} (\tilde{\vartheta}_{,m} J_{mi;\varphi_\alpha}^{-1} J' * 1^* q_i + \tilde{\vartheta}_{,m} J_{mi}^{-1} J'_{;\varphi_\alpha} * 1^* q_i) \delta \varphi_\alpha d\nu^r - \\
& \int_{\partial B^r} \frac{d}{d\tau} (\tilde{\vartheta}^* 1^* q_i J' J_{mi;\varphi_\alpha}^{-1} n_m^r + \tilde{\vartheta}^* 1^* q_i J'_{;\varphi_\alpha} J_{mi}^{-1} n_m^r) \delta \varphi_\alpha da^r + \\
& \int_{B^r} (1^* f_{;E_{kl}} \delta E_{kl} - \tilde{E}_{ij}^* \tilde{S}_{ij;E_{kl}} \delta E_{kl} + \tilde{S}_{kl}^* \delta E_{kl}) J' d\nu^r + \\
& \int_{B^r} (1^* f_{;g_j} \delta g_j + \tilde{g}_i^* \tilde{q}_{i;g_j} \delta g_j - \tilde{g}_j^* \delta g_j) J' d\nu^r + \\
& \int_{A_u^r} (1^* g_{;s_i} \delta s_i + \tilde{s}_i^* \delta u_i) K' da^r + \int_{A_s^r} (1^* g_{;u_i} \delta u_i - \\
& \tilde{u}_i^* \delta s_i) K' da^r + \int_{A_\vartheta} (1^* g_{;q} \delta q^s - \tilde{q}^s \delta q^s) K' da^r + \\
& \int_{A_q} \left[1^* (g_{;\vartheta} + g_{;q} q_{;\vartheta}^p) \delta \vartheta + \tilde{\vartheta}^* (\delta q^s - q_{;\vartheta}^p \delta \vartheta) \right] K' da^r \quad (56)
\end{aligned}$$

where J' , J^{-1} , K' , $J'_{;\varphi_\alpha}$, $K'_{;\varphi_\alpha}$, and $J_{;\varphi_\alpha}^{-1}$ are explicit functions of x' and $x'_{;\varphi_\alpha}$ (see Refs. 18 and 22 for details).

Substitution of Eqs. (46) and (52) and their variations and substitution of Eqs. (35) and (39) as expressed over the reference domain, time differentiation, and some rearrangement gives

$$\begin{aligned}
\delta G^*_{X'} = & \left\{ \int_0^t \int_{B^r} f(u_b, \vartheta, E_{ij}, g_b, S_{ij}, q_b, e, \rho, b_b, r) J'_{;\varphi_\alpha} d\nu^r + \right. \\
& \int_{\partial B^r} g(u_b, s_b, \vartheta, q^s) K'_{;\varphi_\alpha} da^r d\tau + \int_{B^r} \left\{ \tilde{u}_i^* (b_i - \rho \tilde{u}_i) - \right. \\
& \tilde{u}_{i,j} J_{jm}^{-1} * S_{mi} + \tilde{\vartheta}^* (r - \dot{e}) + \tilde{\vartheta}_{,m} J_{mi}^{-1} * q_i \left. \right] J'_{;\varphi_\alpha} + (-\tilde{S}_{ij}^* u_{i,m} - \\
& \tilde{u}_{i,m}^* S_{ji} + \tilde{q}_j^* \vartheta_{,m} + \tilde{\vartheta}_{,m}^* q_j) J_{mj;\varphi_\alpha}^{-1} J' \left. \right\} d\nu^r + \int_{\partial B^r} \tilde{u}_i^* s_i K'_{;\varphi_\alpha} \\
& \times da^r - \int_{\partial B^r} \tilde{\vartheta}^* q^s K'_{;\varphi_\alpha} da^r \left. \right\} \delta \varphi_\alpha + \int_{B^r} \left[1^* f_{;u_i} \delta u_i J' - \right. \\
& \tilde{u}_i^* \rho \delta u_i J' - \tilde{u}_i^* \rho \delta u_i(r, t) J' - \tilde{u}_i^0 \rho \delta v_i(r, t) J' + \\
& (J' J_{mj}^{-1} \tilde{S}_{ij})_{,m}^* \delta u_i \left. \right] d\nu^r - \int_{B^r} \left[1^* (f_{;\vartheta} + f_{;r}; \vartheta + f_{;e}; \vartheta) J' \delta \vartheta + \right. \\
& \tilde{\vartheta}^* r_{;\vartheta} J' \delta \vartheta - \tilde{\vartheta}^* e_{;\vartheta} J' \delta \vartheta - \tilde{\vartheta}^0 e_{;\vartheta}(r, t) J' \delta \vartheta(r, t) - \\
& \tilde{E}_{ij}^* \tilde{S}_{ij;\vartheta} J' \delta \vartheta + \tilde{g}_i^* \tilde{q}_{i;\vartheta} J' \delta \vartheta - (\tilde{q}_i J' J_{mi}^{-1})_{,m}^* \delta \vartheta \left. \right] d\nu^r + \\
& \int_{B^r} \left[1^* f_{;S_{mi}} \delta S_{mi} - \frac{1}{2} (\tilde{u}_{i,j} J_{jm}^{-1} + \tilde{u}_{m,j} J_{ji}^{-1})^* \delta S_{mi} + \right. \\
& \left. \tilde{E}_{mi}^* \delta S_{mi} \right] J' d\nu^r + \int_{B^r} (1^* f_{;q_i} \delta q_i + \tilde{\vartheta}_{,m} J_{mi}^{-1} * \delta q_i -
\end{aligned}$$

$$\begin{aligned}
& \tilde{g}_i^* \delta q_i) J' d\nu^r + \int_{B^r} (1^* f_{;E_{kl}} \delta E_{kl} - \tilde{E}_{ij}^* \tilde{S}_{ij;E_{kl}} \delta E_{kl} + \\
& \tilde{S}_{kl}^* \delta E_{kl}) J' d\nu^r + \int_{B^r} (1^* f_{;g_j} \delta g_j + \tilde{g}_i^* \tilde{q}_{i;g_j} \delta g_j - \tilde{q}_j^* \delta g_j) J' \\
& \times d\nu^r + \int_{A_u^r} (1^* g_{;s_i} \delta s_i + \tilde{u}_i^* \delta s_i) K' da^r + \int_{A_s^r} (1^* g_{;u_i} \delta u_i - \\
& \tilde{s}_i^* \delta u_i) K' da^r + \int_{A_\vartheta} (1^* g_{;q} \delta q^s - \tilde{\vartheta}^* \delta q^s) K' da^r + \\
& \int_{A_q} \left[1^* (g_{;\vartheta} + g_{;q} q_{;\vartheta}^p) \delta \vartheta - \tilde{\vartheta}^* q_{;\vartheta}^p \delta \vartheta + \tilde{q}^s \delta q^s \right] K' da^r \quad (57)
\end{aligned}$$

To eliminate the implicit response field variations in the above equation, the adjoint response fields that correspond to the solution of the problems defined by Eqs. (19–39) (when expressed over the reference domain) can again be used. Once the adjoint problem is solved, the implicit variations are eliminated, and the explicit shape sensitivity is expressed as

$$\begin{aligned}
\delta G_X = & \left\{ \int_0^t \int_{B^r} f(u_b, \vartheta, E_{ij}, g_b, S_{ij}, q_b, e, \rho, b_b, r) J'_{;\varphi_\alpha} d\nu^r + \right. \\
& \int_{\partial B^r} g(u_b, s_b, \vartheta, q^s) K'_{;\varphi_\alpha} da^r d\tau + \int_{B^r} \left\{ \tilde{u}_i^* (b_i - \right. \\
& \rho \tilde{u}_i) - \tilde{u}_{i,j} J_{jm}^{-1} * S_{mi} + \tilde{\vartheta}^* (r - \dot{e}) + \tilde{\vartheta}_{,m} J_{mi}^{-1} * q_i \left. \right] J'_{;\varphi_\alpha} + \\
& (-\tilde{S}_{ij}^* u_{i,m} - \tilde{u}_{i,m}^* S_{ji} + \tilde{q}_j^* \vartheta_{,m} + \tilde{\vartheta}_{,m}^* q_j) J_{mj;\varphi_\alpha}^{-1} J' \left. \right\} \\
& \times d\nu^r + \int_{\partial B^r} \tilde{u}_i^* s_i K'_{;\varphi_\alpha} da^r - \int_{\partial B^r} \tilde{\vartheta}^* q^s K'_{;\varphi_\alpha} da^r \left. \right\} \delta \varphi_\alpha \quad (58)
\end{aligned}$$

The above results are consistent with those appearing in Refs. 16–18 and 21. In Refs. 5, 9 and 10, the boundary version of the material derivative method is utilized to obtain explicit shape sensitivities. As seen in Ref. 10, special treatment is required when applying this technique to problems with material interfaces or discontinuous boundary conditions. These problems do not arise when the domain version of the material derivative method is used.³⁷ In the present formulation, the material properties and boundary conditions are assumed to be continuous. However, discontinuities can be handled by subdividing B^r into fixed subregions with continuous material properties and boundary data and restricting x to map them into the corresponding regions of B . This is demonstrated in the example problem.

V. Linearization

Finite element techniques which incorporate the Newton-Raphson iteration method to determine the real response can be utilized to solve the adjoint response and to evaluate the sensitivities.

The tangent constitutive relations are defined

$$C_{ijkl} \equiv \tilde{S}_{ij;E_{kl}} \quad (59)$$

$$M_{ij} \equiv \tilde{S}_{ij;\vartheta} \quad (60)$$

$$K_{ij} \equiv \tilde{q}_{i;g_j} \quad (61)$$

$$c \equiv e_{;\vartheta} \quad (62)$$

where $C(E, \vartheta, \phi)$, $M(\vartheta, \phi)$, $K(\vartheta, \phi)$, and $c(\vartheta, \phi)$ are the tangential stress-strain tensor, stress-temperature tensor, conductivity tensor, and specific heat, respectively. These tangential

relationships are used to express Eqs. (26), (34), (36), (38), and (40) as

$$\begin{aligned} \bar{F}(x, t - \tau) = & f_{;\vartheta} |_{(x, \tau)} + f_{;r'} |_{(x, \tau)} r'_{;\vartheta} |_{(x, \tau)} + f_{;e'} |_{(x, \tau)} c' |_{(x, \tau)} - \\ & \bar{E}_{ij}(x, t - \tau) (C'_{ijkl;\vartheta} |_{(x, \tau)} E_{kl}(x, \tau) + M'_{ij} |_{(x, \tau)} + \\ & \vartheta(x, \tau) M'_{ij;\vartheta} |_{(x, \tau)}) \quad \text{in } B \times [0, t] \end{aligned} \quad (63)$$

$$\begin{aligned} \bar{S}_{kl}(x, t - \tau) = & \bar{E}_{ij}(x, t - \tau) C'_{ijkl} |_{(x, \tau)} + \\ & \bar{S}_{kl}^A(x, t - \tau) \quad \text{in } B \times [0, t] \end{aligned} \quad (64)$$

$$\begin{aligned} -\bar{q}_{i,i}(x, t - \tau) + \bar{\vartheta}(x, t - \tau) r'_{;\vartheta} |_{(x, \tau)} - \\ \bar{g}_i(x, t - \tau) K'_{ij;\vartheta} |_{(x, \tau)} g_j(x, \tau) + \bar{f}(x, t - \tau) = \\ \bar{\vartheta}(x, t - \tau) c' |_{(x, \tau)} \quad \text{in } B \times [0, t] \end{aligned} \quad (65)$$

$$\begin{aligned} \bar{q}_j(x, t - \tau) = -\bar{g}_i(x, t - \tau) K'_{ij} |_{(x, \tau)} + \\ \bar{q}_j^A(x, t - \tau) \quad \text{in } B \times [0, t] \end{aligned} \quad (66)$$

$$\begin{aligned} \delta G_D = & \left\{ \int_0^t \int_B (f'_{;e'} e'_{;\vartheta} + f'_{;\rho} \rho'_{;\vartheta} + f'_{;b_i} b'_{i;\vartheta} + f'_{;r'} r'_{;\vartheta}) d\nu \right. \\ & + \int_{A_u} g_{;u p'} u'_{i;\vartheta} da + \int_{A_s} g_{;s p'} s'_{i;\vartheta} da + \int_{A_\vartheta} g_{;\vartheta p'} \vartheta'_{;\vartheta} da + \\ & \left. \int_{A_q} g_{;q p'} q'_{;\vartheta} da \right\} d\tau + \int_B \left[\bar{u}_i^* (b'_{i;\vartheta} - \rho'_{;\vartheta} \bar{u}_i) + \right. \\ & \bar{u}_i(x, t) \rho' u'_{i;\vartheta} + \bar{u}_i(x, t) \rho' v'_{i;\vartheta} + \bar{\vartheta}^* (r'_{;\vartheta} - e'_{;\vartheta}) + \\ & \bar{\vartheta}(x, t) c^0 \vartheta'_{;\vartheta} - \bar{E}_{ij}^* (C'_{ijkl;\vartheta} E_{kl} + \vartheta M'_{ij;\vartheta}) - \bar{g}_i^* K'_{ij;\vartheta} g_j \Big] d\nu \\ & - \int_{A_u} \bar{s}_i^* u'_{i;\vartheta} da + \int_{A_s} \bar{u}_i^* s'_{i;\vartheta} da + \\ & \left. \int_{A_\vartheta} \bar{q}^* \vartheta'_{;\vartheta} da - \int_{A_q} \bar{\vartheta}^* q'_{;\vartheta} da \right\} \delta \vartheta_\alpha \end{aligned} \quad (67)$$

where $c^0 \equiv e'_{;\vartheta}$.

VI. Example Problem

In this example problem, the finite element method is used to calculate the real response, adjoint response, and shape sensitivities for a tank design problem. The finite element formulation uses the full Newton-Raphson technique³⁴ to obtain the thermal response. The nonsymmetric tangent stiffness matrix and implicit time integration schemes are used. The elastic response is evaluated in the usual elastostatic linear manner; however, due to the dependence of \bar{S} on temperature, both C and M [see Eqs. (59) and (60)] vary with location and time. The tank is modeled as a nonlinear, uncoupled, quasistatic, thermoelastic system. Approximate finite-difference sensitivities are computed to validate the explicit adjoint sensitivity analysis.

Consider the holding tank and nozzle in Fig. 1. Initially, the structure is near steady state with a uniform temperature of 345°C. Then a flow of cold water surges into the tank. This sudden cooling creates large thermal stresses, which are especially prevalent in the nozzle (region A of Fig. 1), where the protective shield which lines the nozzle contacts the tank.

Only region A is considered in the model, and axisymmetry is used to reduce the computational expense. The finite element mesh appears in Fig. 2. It consists of 145 8-node quadrilateral elements and 528 nodes. Zero vertical displacement and zero heat flux constraints are enforced along the bottom edge of the model. The top edge of the model is prescribed to have zero heat flux. The density of the shield is 7850 Kg/m³. The modulus of elasticity, coefficient of thermal expansion, thermal conductivity, and specific heat of the shield are temperature-dependent, as seen in Figs. 3-6. (Here, enthalpy is modeled as piecewise linear. Hence, the specific heat appears as a series of step functions.) The density for the remainder of the tank is 7800 Kg/m³. Other properties for this region are displayed in Figs. 3-6. The Poisson's ratio for both materials is 0.3. The water temperature is initially 345°C. It is then dropped linearly to 288°C over a period of 45 s and raised again in the same fashion. The temperature of the air which cools the exterior of the tank is held constant at 30°C. Convection coefficients are 35000 W/m²°C for the surface of the shield that contacts the incoming water, 267 W/m²°C on the remainder of the tank's interior, and 5 W/m²°C on the tank's exterior. The reference temperature is 0°C. Uniform time increments of 3 s are used for a total analysis period of 90 s.

The results of the analysis are displayed in Figs. 7-8. These contour plots depict the algebraic maximum of the principle stresses at $\tau = 42$ s and $\tau = 84$ s, the times at which this stress obtains its minimum and maximum magnitudes, respectively. This stress measure can be used in design criteria for holding tanks. A large variation in this stress measure is known to be related to fatigue failures.

A shape sensitivity analysis is performed to determine how shape alterations will affect this stress measure. In particular, the stresses at location X (see Fig. 2) are investigated. The largest stress variation, 500.9 MPa, is present at this point. G_1 is defined to model this stress measure as

$$G_1 = G_{42} - G_{84} \quad (68)$$

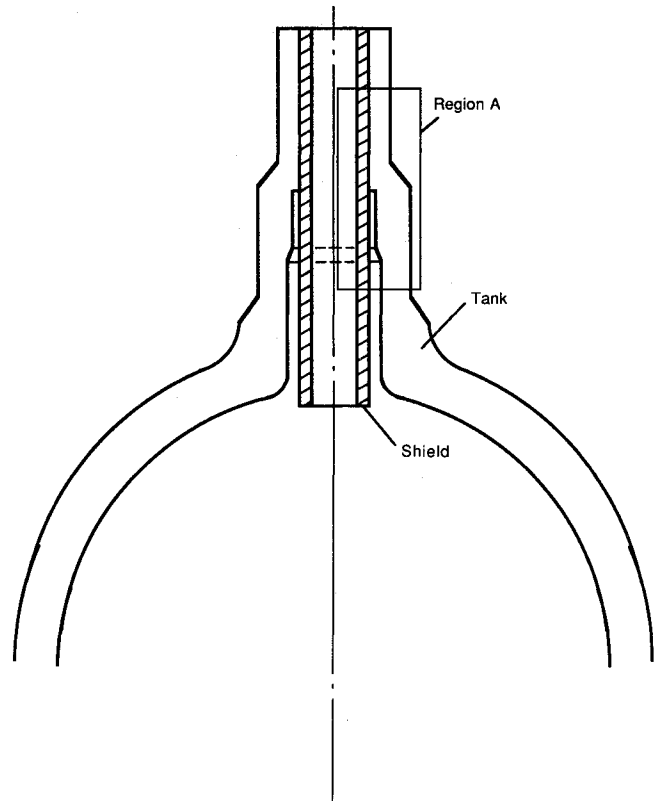


Fig. 1 Holding tank.

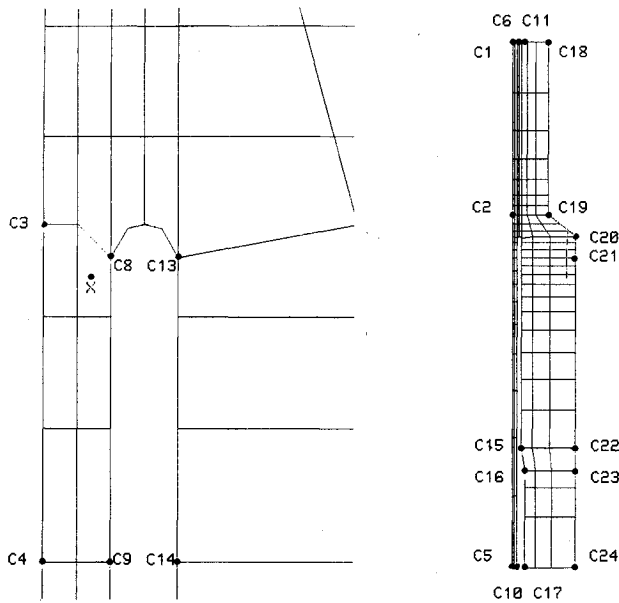


Fig. 2 Holding tank model.

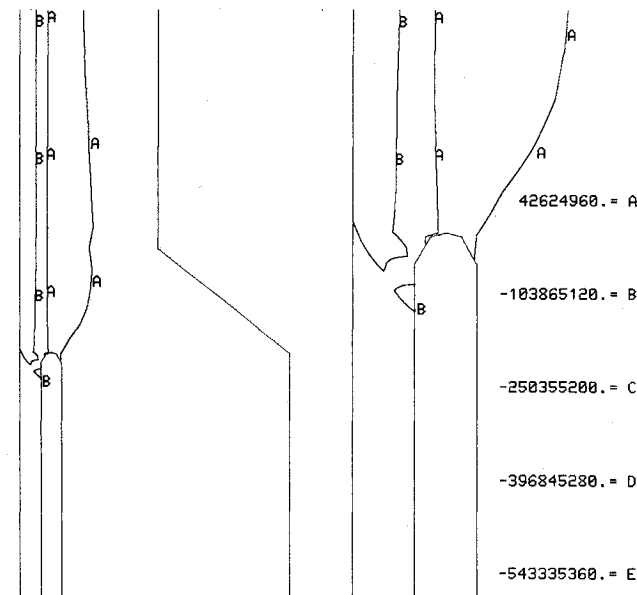


Fig. 3 Elastic modulus vs temperature.

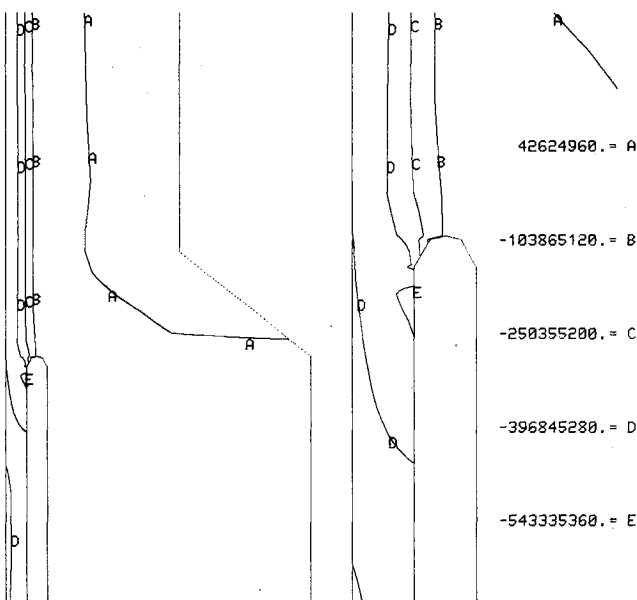


Fig. 4 Thermal expansion coefficient vs temperature.

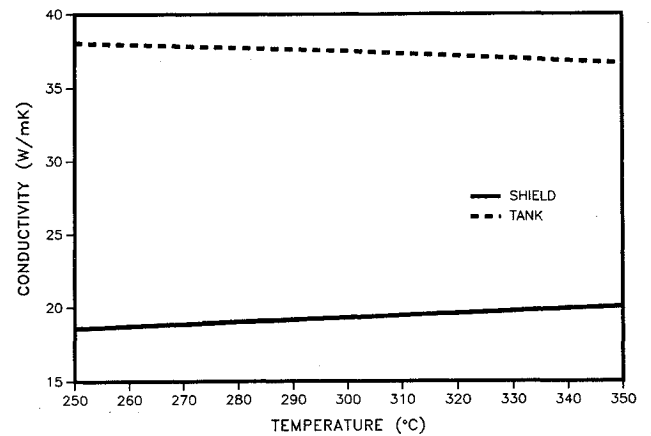


Fig. 5 Specific heat vs temperature.

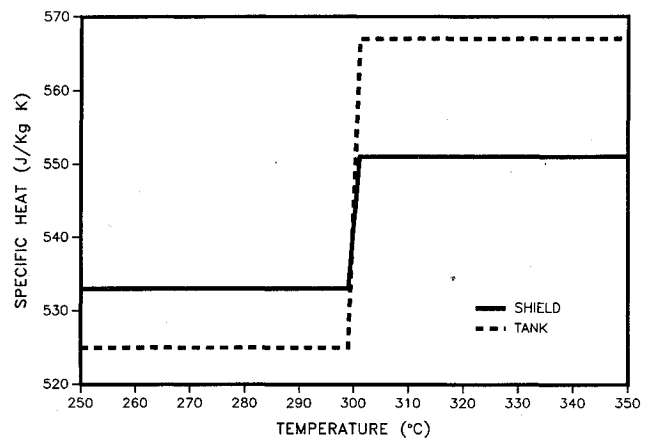


Fig. 6 Thermal conductivity vs temperature.

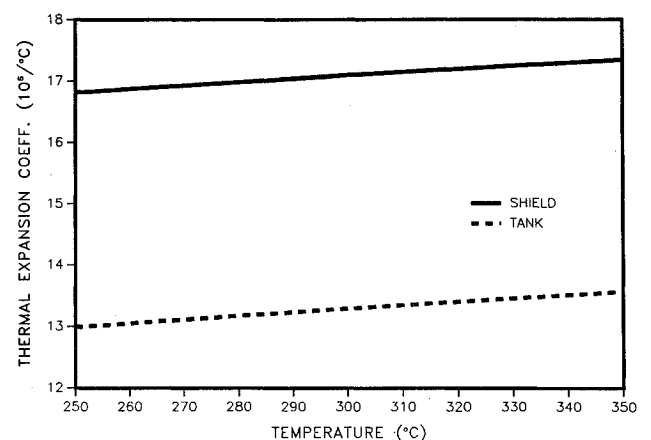


Fig. 7 Stress contours at 42 s.

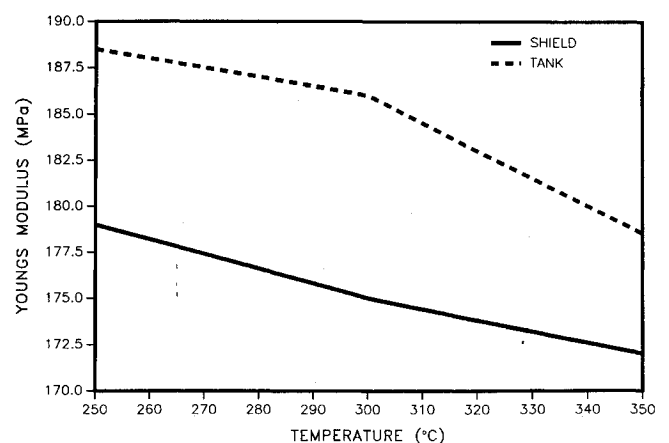


Fig. 8 Stress contours at 42 s.

where

$$G_{42} = \begin{cases} \frac{1}{3} \int_{39}^{42} \int_B \delta(x-X) S_1 d\nu d\tau & \text{if } |S_1| = \max(|S_1|, |S_2|, |S_3|) \text{ at } \tau=42 \\ \frac{1}{3} \int_{39}^{42} \int_B \delta(x-X) S_2 d\nu d\tau & \text{if } |S_2| = \max(|S_1|, |S_2|, |S_3|) \text{ at } \tau=42 \\ \frac{1}{3} \int_{39}^{42} \int_B \delta(x-X) S_3 d\nu d\tau & \text{if } |S_3| = \max(|S_1|, |S_2|, |S_3|) \text{ at } \tau=42 \end{cases} \quad (69)$$

$$G_{84} = \begin{cases} \frac{1}{3} \int_{81}^{84} \int_B \delta(x-X) S_1 d\nu d\tau & \text{if } |S_1| = \max(|S_1|, |S_2|, |S_3|) \text{ at } \tau=84 \\ \frac{1}{3} \int_{81}^{84} \int_B \delta(x-X) S_2 d\nu d\tau & \text{if } |S_2| = \max(|S_1|, |S_2|, |S_3|) \text{ at } \tau=84 \\ \frac{1}{3} \int_{81}^{84} \int_B \delta(x-X) S_3 d\nu d\tau & \text{if } |S_3| = \max(|S_1|, |S_2|, |S_3|) \text{ at } \tau=84 \end{cases} \quad (70)$$

and

$$S_1 = [-b + (b^2 - 4c)^{1/2}] / 2 \quad (71)$$

$$S_2 = [-b - (b^2 - 4c)^{1/2}] / 2 \quad (72)$$

$$S_3 = S_{33} \quad (73)$$

in which $b = -(S_{11} + S_{22})$; $c = -S_{12}^2$; and $\delta(\cdot)$ is the Dirac delta function. The fraction $1/3$ is used to normalize the functional value over the time interval. This normalization is one method to approximate Dirac delta functions defined on the time domain when numerical integration schemes are employed.^{18,20-22}

Recalling the time shift in Eq. (20) and noting Eqs. (68-73), the data for the adjoint elastic analyses are defined as

$$\tilde{E}_{11}^A, \tilde{E}_{22}^A = \begin{cases} -\frac{1}{3} \delta(x-X)(1-b)/(2d) & \text{if } S_1 = G_{84} \text{ and } \tau \in [6,9] \\ \frac{1}{3} \delta(x-X)(1-b)/(2d) & \text{if } S_1 = G_{42} \text{ and } \tau \in [48,51] \\ -\frac{1}{3} \delta(x+X)(1+b)/(2d) & \text{if } S_2 = G_{84} \text{ and } \tau \in [6,9] \\ \frac{1}{3} \delta(x+X)(1+b)/(2d) & \text{if } S_2 = G_{42} \text{ and } \tau \in [48,51] \\ 0 & \text{otherwise} \end{cases} \quad (74)$$

$$\tilde{E}_{12}^A = \begin{cases} -\frac{1}{3} \delta(x-X) 2 S_{12} / d & \text{if } S_1 = G_{84} \text{ and } \tau \in [6,9] \\ \frac{1}{3} \delta(x-X) 2 S_{12} / d & \text{if } S_1 = G_{42} \text{ and } \tau \in [48,51] \\ -\frac{1}{3} \delta(x-X) 2 S_{12} / d & \text{if } S_2 = G_{84} \text{ and } \tau \in [6,9] \\ \frac{1}{3} \delta(x-X) 2 S_{12} / d & \text{if } S_2 = G_{42} \text{ and } \tau \in [48,51] \\ 0 & \text{otherwise} \end{cases} \quad (75)$$

$$\tilde{E}_{33}^A = \begin{cases} -\frac{1}{3} \delta(x-X) & \text{if } S_3 = G_{84} \text{ and } \tau \in [6,9] \\ \frac{1}{3} \delta(x-X) & \text{if } S_3 = G_{42} \text{ and } \tau \in [48,51] \\ 0 & \text{otherwise} \end{cases} \quad (76)$$

where $d = (b^2 - 4c)^{1/2}$.

The adjoint thermal data consist solely of the term $\tilde{r}(x, \tau - t) = \tilde{E}_{ij}(x, t - \tau) (C_{ijkl} \vartheta|_{(x,\tau)} E_{kl}(x, \tau) + M'_{ij} \vartheta|_{(x,\tau)} + \vartheta|_{(x,\tau)})$ [see Eq. (63)]. Upon the determination of the adjoint response, the shape sensitivities with respect to each nodal coordinate are found by evaluating

$$\delta G_X = \left\{ \int_0^t \int_{B^r} f(u_b, \vartheta, E_{ij}, g_b, S_{ij}, q_b, e, \rho, b_b, r) (J'_{;\varphi_\alpha} R' + J' R'_{;\varphi_\alpha}) d\nu' + \int_{\partial B^r} g(u_b, S_b, \vartheta, q^s) (K'_{;\varphi_\alpha} R' + K' R'_{;\varphi_\alpha}) da' \right\} \times d\tau + \int_{B^r} \left\{ \tilde{u}_i^* (b_i - \rho \tilde{u}_i) - \tilde{u}_{i,j} J_{jm}^{-1} S_{mi} + \tilde{\vartheta}^* (r - \right.$$

$$\left. \tilde{e}) + \tilde{\vartheta}_{,m} J_{mi}^{-1} q_i \right\} (J'_{;\varphi_\alpha} R' + J' R'_{;\varphi_\alpha}) + (-\tilde{S}_{ij}^* u_{i,m} - \tilde{u}_{i,m}^* \times S_{ji} + \tilde{q}_j^* \vartheta_{,m} + \tilde{\vartheta}_{,m}^* q_j) J_{mj;\varphi_\alpha}^{-1} J' R' \Big\} d\nu' + \int_{\partial B^r} \tilde{u}_i^* s_i (K'_{;\varphi_\alpha} R' + K' R'_{;\varphi_\alpha}) da' - \int_{\partial B^r} \tilde{\vartheta}^* q^s (K'_{;\varphi_\alpha} R' + K' R'_{;\varphi_\alpha}) da' \Big\} \delta \varphi_\alpha \quad (77)$$

This equation results from the transformation of Eq. (58) to cylindrical coordinates (see Ref. 35). In the above, $R(r, \varphi_\alpha) =$

x_i ; i.e., the radial position; J is the transpose of the isoparametric Jacobian matrix; and all Arabic indices range from 1 to 2.

In this analysis, a boundary parameterization scheme is used³⁸ to represent the shape of the structure. Here, 22 surface control points are used to linearly constrain the nodes which lie between them. The sensitivities with respect to the control point coordinates are then calculated from the node coordinate sensitivities using the chain rule. The results of the sensitivity analyses appear in Table 1, in which the second column lists the explicit sensitivities (computed by the present adjoint formulation) with respect to the selected control point coordinates. Only motions of the exterior control points in close proximity to X that yield true shape changes are considered to be variable in this analysis. Specifically, radial (x -direction) movements of points C_2 , C_3 , C_4 , C_{19} , C_{20} , and C_{21} and axial (z -direction) movements of points C_{19} and C_{21} are considered.

As seen from the tabulated values, control points C_2 , C_3 , C_{19} , C_{20} , and C_{21} should be moved radially inward and C_4 radially outward to decrease the stress variation. A decrease in G_1 will also result if points C_{19} and C_{20} are displaced downward. It is further noted that the sensitivity with respect to movements of points C_3 and C_4 is much greater than the sensitivity with respect to the other control point movements.

To validate the sensitivity analysis, finite-difference calculations were performed. In each of these calculations, a control point coordinate is perturbed, the structure is reanalyzed, and the sensitivity is approximated as the difference between the perturbed and original values of G_1 divided by the value of the perturbation. The finite-difference approximations for differential increments of 1×10^{-4} m, 1×10^{-5} m, and 1×10^{-6} m appear in columns 3, 5, and 7 of Table 1, respectively. The percentage difference between the adjoint and finite-difference sensitivity values are given in columns 4, 6, and 8. For control points 3 and 4, the results are reasonably insensitive to the perturbation size and are in agreement with the sensitivities calculated via the adjoint method. The finite-difference results for the other points are sensitive to the perturbation size. This is possibly due to roundoff error because the magnitudes of these sensitivities are much less than those associated with points 3 and 4. Errors can also be attributed to convergence tolerance in the Newton-Raphson termination criterion. This example illustrates how the magnitude of the finite-difference perturbations can affect the accuracy of the sensitivity approximation. None of these accuracy problems are a concern when the explicit adjoint method is used.

The times required to perform the analysis of the real system, evaluate the shape sensitivities, and compute the functional value were 114, 83, and 0.4 cpu s, respectively. In this example, the method of storing the decomposed stiffness matrices to expedite the adjoint analyses was not used due to the large storage requirements. However, the 83 s required to calculate the sensitivities via the adjoint method was still much less than the 916 s (eight additional analyses and functional evaluations) required when using the finite-difference method. Here, the 916 s required for the finite-difference computations accounts for only one differential increment. The total time required to compute the finite-difference approximations

(three increment sizes required in this example to obtain accurate approximations) was 2748 s. This cost variance is attributed to the efficiency of the adjoint technique as compared to the finite-difference method in nonlinear problems and in problems with relatively few design functionals. The question of which formulation is most efficient depends on the number of design parameters and design functionals. In the adjoint method, one additional linear problem must be solved for each design functional. (The decomposed stiffness matrix can be made available to further reduce this computational expense.) The finite-difference approach requires a full nonlinear reanalysis for each independent design parameter. (This reanalysis expense can be reduced if the real response from the original analysis is used as the starting point in the Newton-Raphson iteration.) This point is illustrated in the present example. For each additional control point, the finite-difference computational expense increases by 114.4 s per increment (one nonlinear analysis and one functional evaluation), while the adjoint computational expense remains unchanged. For each additional design functional, the adjoint cost increases by 83 s, whereas the finite-difference cost increases slightly (one functional evaluation or 0.4 s). All calculations were performed on a single processor of a CRAY X-MP computer.

VII. Conclusion

Explicit sensitivities for nonlinear, uncoupled, dynamic thermoelastic systems have been presented. In the formulation, the variation of a general design functional is expressed in explicit form with respect to perturbations of the design fields and structural shape. The derivation utilizes the Lagrange multiplier method (which requires no a priori knowledge of the adjoint governing equations), the convolution (which eliminates the need for time mappings in the adjoint problem), and domain parameterization (which easily treats problems with material interfaces and discontinuous boundary data).

In an example problem, the computational advantages of the explicit method over the finite-difference method are illustrated. The inability of the finite-difference method to converge to a clear limiting value is shown. The adjoint method presented here does not suffer this problem. The general agreement between the explicit adjoint sensitivities and finite-difference sensitivities indicate that accurate sensitivities for the finite-element model were obtained. As is always the case, the analyst must ensure that the finite-element solution is sufficiently accurate so that the computed sensitivities are meaningful.

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Table 1 Design sensitivities, δG_1

Control point coordinate	Adjoint method ($\times 10^9$ Pa/m)	Finite-difference method ($\times 10^9$ Pa/m)					
		$\Delta = 0.0001$	$\Delta \%$	$\Delta = 0.00001$	$\Delta \%$	$\Delta = 0.000001$	$\Delta \%$
C_2x	0.32964	0.33013	-1.5	0.32623	1.0	0.20216	39
C_3x	17.854	18.161	-1.7	17.817	0.20	17.787	0.38
C_4x	-25.978	-26.182	-3.2	-26.108	-0.50	-26.163	-7.1
$C_{19}x$	1.8692	1.8657	0.19	1.8554	0.74	1.7309	7.4
$C_{19}y$	5.3240	5.3098	0.27	5.1862	2.6	3.9388	26
$C_{20}x$	0.21172	0.21000	0.81	0.19782	6.6	0.073131	66
$C_{20}y$	0.16307	0.16185	0.75	0.14927	8.5	0.024538	85
$C_{21}x$	0.14173	0.14027	1.0	0.12784	9.8	0.0032249	98

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