Review

Optimal Design of Structures under Impact Loading

Uwe Schramm
Walter D. Pilkey
The University of Virginia
Department of Mechanical, Aerospace, and Nuclear Engineering
Thornton Hall, Charlottesville, VA 22903-2442

In the design process structural optimization is a useful tool to reach design decisions. The impact behavior of structures is important for many designs, such as for automobiles. This article reviews methodology for the optimization of structures under impact loading. The optimization problem is to minimize the structural mass with constraints on the transient dynamic response of the structure. The structural behavior is nonlinear dynamic. Optimization is performed using the approximation concept. Design sensitivity analysis for transient response is treated.

INTRODUCTION

The layout of structures is influenced by many decisions. The behavior of the structure is complex and so is the design process. Structural optimization is a useful tool for structural design. Here the complexity of the layout can be described mathematically and the decision process can be supported. Often optimization of structural elements can lead to significant cost reductions. In this study, the optimization of structures under impact loading is considered. Research in this field is especially important for automobile design where crashworthiness is a vital area that influences design decisions.

The design problem is given in the form of an optimization problem. Optimization of the structure can be performed to obtain a certain structural response and to make the structural mass as low as possible. In the case where the solution of the mass minimization does not yield a predefined performance limit, the structure will be optimized with that mass as a constraint to obtain a response as close as possible to that prescribed. The structural optimization problem may be expressed as

Objective function:	$W(\mathbf{p}) \Rightarrow \min,$
Subject to the state equation	$\mathbf{P}\dot{\mathbf{u}} = \mathbf{f}(\mathbf{u}, \mathbf{p}, t),$ $0 \leq t \leq t_e$
with the initial conditions	$\mathbf{u}(0) = \mathbf{u}_0,$
Inequality constraints:	$\mathbf{g}(\mathbf{u}, \mathbf{p}, t) \leq \mathbf{0}$
Equality constraints:	$\mathbf{h}(\mathbf{p}) = \mathbf{0}$
Side constraints:	$\mathbf{p}^l \leq \mathbf{p} \leq \mathbf{p}^u.$ (1)

The objective function W is the total or a weighted mass of the structure. Functions $g_i \in \mathbf{g}$ are structural responses. In the second case mentioned above, the structural response would be the objective function and the structural mass the constraint. The state equation describes the dynamic behavior of the structure that is to be optimized. It is the first-order form of the governing equations of motion of the structure. The state

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vector **u** contains the generalized displacements and velocities. The quantity **f** is the load vector.

The quantity $\mathbf{p} = \{p_j\}$, $j = 1, \ldots, n_p$ is the vector of design variables. The vectors $\mathbf{p}^l$ and $\mathbf{p}^u$ are the lower and upper bounds on the design variables, respectively. The equality constraints are constraints on the design variables that are independent on the time. Depending on the type of design variables, the structural optimization problem can be one of sizing or shape optimization. For the first type, the design variables are input parameters of structural elements such as beam cross-sectional properties or plate thicknesses; for the second type, the design variables are control variables of the geometry of the structure. A third type of structural optimization problem that will not be considered here is known as topology optimization. There, the design variables determine the material distribution in the structure.

Optimization of structures in a crash environment is a challenging subject. The structural behavior is considered to be nonlinear dynamic. The structural optimization problem of Eq. (1) is also nonlinear, and it does not have any special simplifying characteristics. Research on structural optimization using numerical methods has been conducted for some time. Methodology for linear and nonlinear structures has been developed. However, structural optimization for nonlinear problems is a relatively young field, especially for complex structures and dynamic problems.

This exposition begins with a review of past work in the field of structural optimization, including constraints involving the dynamic response and nonlinear behavior of structures. Based on the literature review, methodology for a design sensitivity analysis is given that can be applied for structural optimization in a crash environment.

LITERATURE REVIEW

In the three and a half decades since the appearance of the paper by Schmit (1960), structural optimization using numerical tools has advanced to become an important field in applied and computational mechanics. Today many practicing engineers apply optimization tools to determine design improvements using the results of structural analyses. Numerous articles have been written in this field. Several review articles have appeared (Vanderplaats, 1982; Haftka and Grandhi, 1986; Levy and Lev, 1987; Arora, 1990). The latest state-of-the-art studies on structural optimization can be found in the books edited by Kamat (1993) and Herskovits (1995). Structural optimization is already implemented in several commercial and academic finite element codes (Duysinx and Fleury, 1993; Johnson, 1993).

This short review will focus on structural optimization technology that is available for the optimization of structures under impact loading. Structural optimization related to dynamic response was considered as early as 1970 (Fox and Kapoor, 1970). Since then many studies have been conducted to establish techniques for dynamic response optimization (Feng et al., 1977; Haug and Arora, 1979; Hsieh and Arora, 1984, 1985a,b; Tseng and Arora, 1989; Tortorelli et al., 1990; Choi and Wang, 1993; Bucher and Braun, 1994a,b; Chahande and Arora, 1994). Some practical applications for structural optimization in crashworthiness design are available in the automobile industry literature and are based on concept models (Song, 1986; DeVries et al., 1986; Pant and Cheng, 1995). A concept model is a rigid body system used for preliminary design decisions.

The solution of structural optimization methods is mostly accomplished using approximation techniques. Approximation methods approach the solution of the design optimization problem by establishing approximations to the actual design optimization problem that can be solved easier. A detailed review on approximation concepts was published by Barthelemy and Haftka (1993).

The most popular computational techniques for the solution of structural optimization problems are methods that use local approximations of the objective function and constraints (Schmit and Farshi, 1974; Schmit and Fleury, 1980). In such methods the optimization problem is approximated at a single point of the design space. The solution of the approximate optimization problem determines another point in the design space where then again an approximate optimization problem is formed. This process is continued until convergence. The algorithm involves the following solution steps: 1. structural analysis; 2. stop if optimum is reached; 3. design sensitivity analysis; 4. solution of an approximate optimization problem; 5. back to 1. The design sensitivity analysis provides the derivatives of the structural behavior with respect to the design variables using the results of the structural analysis. An approximation of the objective function and the constraints at the actual optimization step are found using the design sensitivity information. The result is a local approximation of the design optimization problem that can be solved using methods of linear or nonlinear programming. It is assumed that in each optimization step only small changes of the structure occur, and hence, sequential solution of approximate optimization problems can lead to an overall convergence of the solution of the structural optimization problem. Although the assumption of small changes cannot always be retained, local approximation methods have been successfully applied to a variety of structural optimization problems. The simplest way to establish a local approximation appears to be to form a linear optimization problem using first-order design sensitivity (Zienkiewicz and Campbell, 1973). Other methods based on first-order sensitivity information include reciprocal approximation (Storaasli and Sobieszczanski–Sobieski, 1974) and conservative approximation (Starnes and Haftka, 1979). The latter technique, which is sometimes called convex linearization, forms a convex separable optimization problem. From the convex approximation, special optimization algorithms have been developed, such as methodology based on the duality of convex optimization problems (Braibant and Fleury, 1985) and the method of moving asymptotes (Svanberg, 1987). Higher order sensitivity information can be used to improve local approximations (Fleury, 1989).

Other approximation techniques that can be characterized as global approximation methods include the response surface approach, where an analytical response surface is established using numerical experiments that can be searched for an optimal design, and approximations by neural networks (Hajela and Berke, 1992). For a more detailed review on such methods see Barthelemy and Haftka (1993).

Methodology for the analysis of complex structures under dynamic loading is well established. For complex structures finite elements are used (Jones and Wierzbicki, 1983; Haug et al., 1983; Bathe et al., 1975; Bathe, 1995). Commercial software packages, such as DYNA3D (Hallquist, 1993) and ABAQUS (1989), are available for the solution of nonlinear dynamic problems.

A crucial ingredient for optimization applications is the sensitivity analysis that provides the gradient of the response functions with respect to the design variables. The principles of design sensitivity analysis can be found in several texts and review articles (Adelmann and Haftka, 1986; Haug et al., 1986; Haftka and Adelmann, 1989; Haftka et al., 1990; Arora, 1995). Design sensitivity analyses for dynamic response using direct differentiation and adjoint variable methods have been developed (Feng et al., 1977; Hsieh and Arora, 1984). Also available is a method based on Green's functions (Demirlap and Rabitz, 1981). Computational aspects of sensitivity analysis for linear transient response have been discussed by Greene and Haftka (1991). Design sensitivity analysis for transient response is usually based on first-order state equations. In such a form the methodology would also be applicable to nonlinear structures (Hsieh and Arora, 1984). Methodology for shape optimization and dynamic structures based on a continuum approach has been developed (Meric, 1988; Tortorelli et al., 1990). All methods cited previously are derived in the time domain. Wang and Lu (1995) introduced a method for linear transient response in the frequency domain.

In connection with impact loading, the sensitivity analysis for nonlinear structures is of interest. Sensitivity analyses for such problems have been studied since the late 1980s (Mroz et al., 1985; Ryu et al., 1985; Choi and Santos, 1987). A variational theory for the design sensitivity analysis of nonlinear static systems has been developed (Cardoso and Arora, 1988; Tsay and Arora, 1990a,b). Some work has been done recently in the field of nonlinear dynamics. Cardoso and Arora (1992) gave a unified variational theory for design sensitivity analysis for nonlinear dynamic response that includes sizing and shape design variables. A design sensitivity analysis for nonlinear dynamic response with viscoplastic material was presented by Kulkarni and Noor (1995).

It is important in connection with structural optimization to consider the implementation of such methods. Two ways are possible, both having advantages and disadvantages. On the one hand, the sensitivity analysis and optimization could be implemented separately. The advantage of such an approach would be that a sensitivity analysis and optimization tool could be combined with several analysis codes. However, the development costs would be very high and the resulting tool might not be very efficient. On the other hand, a sensitivity analysis and optimization could be implemented directly into an analysis code. In this case one would need access to the source code, but the result could be very efficient. Another disadvantage would be that the development would not be transferable to other analyzers. Both approaches with respect to nonlinear finite element codes are discussed by Arora and Cardoso (1989) and Poldneff et al. (1993).

Very recently, topology optimization has also been applied to structural optimization of dynamic problems (Ma et al., 1993, 1995; Kikuchi et al., 1995). The topology optimization approach is not yet applicable to complex structures. Also, pointwise constraints such as stresses cannot be applied.

STRUCTURAL OPTIMIZATION

The structural optimization problem is given by Eq. (1). Objective and constraint functions are performance measures of the structural system. In contrast to steady-state response problems, for transient response problems these functions depend on time. Three types of constraints can be distinguished:

1. Pointwise constraints:

$$g_i(\mathbf{u}, \mathbf{p}, t) = \bar{\psi}_k(\mathbf{u}, \mathbf{p}, t) \leq 0, \quad k = 1, \ldots, n_k, \quad 0 \leq t \leq t_e. \tag{2}$$

   These constraints can be displacements, velocities, accelerations, or stresses at specific points of the structure. It is assumed that these constraints are satisfied for each time of the solution. Because the functions of Eq. (2) have to be discretized for each time step, there tends to be a large number of constraints.

2. Integral type constraints:

$$g_i(\mathbf{u}, \mathbf{p}) = \int_0^{t_e} \psi_l(\mathbf{u}, \mathbf{p}, t)dt \leq 0, \quad l = 1, \ldots, n_l, \quad 0 \leq t \leq t_e. \tag{3}$$

   These constraints, which are computed over a specified time interval, can be performance measures such as injury criteria or the amount of storable energy.

3. Explicit constraints on the design variables:

$$\mathbf{h}(\mathbf{p}) = \mathbf{0}, \tag{4}$$

$$\mathbf{p}^l \leq \mathbf{p} \leq \mathbf{p}^u. \tag{5}$$

   These constraints follow from geometric considerations of the design such as dependencies of design variables and limits on the design variables. Equality constraints are often eliminated. On one hand, this can be accomplished by transforming them into two inequality constraints. On the other hand, if the constraints of Eq. (4) describe the linking of design variables, they are linearized and removed using a condensation process. This eliminates some design variables, which is advantageous for the numerical efficiency.

For the solution of the optimization problem it is desirable to express the constraints of Eq. (2) in integral form. This would remove the time dependence and therefore considerably reduce the number of constraints. One way to eliminate the time dependence from the pointwise constraints would be to simply average the constraints over a time interval. This could be disadvantageous because the averaging could suppress critical constraints. Another method is the introduction of critical point constraints (Hsieh and Arora, 1984). This means that only the critical values of the constraints are considered. Let t_c be the time when the constraint $\bar{\psi}_k(\mathbf{u}, \mathbf{p}, t)$ becomes critical. Then the constraint of Eq. (2) can be written in integral form as

$$g_i(\mathbf{u}, \mathbf{p}) = \int_0^{t_e} \bar{\psi}_k(\mathbf{u}, \mathbf{p}, t)\delta(t - t_c)dt \leq 0. \tag{6}$$

Due to the nonlinear character of the structural optimization problem of Eq. (1), the solution of the optimization problem must be obtained iteratively. This is effectively accomplished using local function approximations. Figure 1 shows the solution scheme. In each iteration step s the approximation

$$\tilde{W}^{(s+1)}(\mathbf{p}) \Rightarrow \min, \tag{7}$$

$$\tilde{g}_i^{(s+1)}(\mathbf{p}) \leq 0, \quad i = 1, \ldots, n_c,$$

$$\mathbf{p}^l \leq \mathbf{p} \leq \mathbf{p}^u, \tag{8}$$

of the design optimization problem of Eq. (1) is being solved. The tilde indicates the approxima-

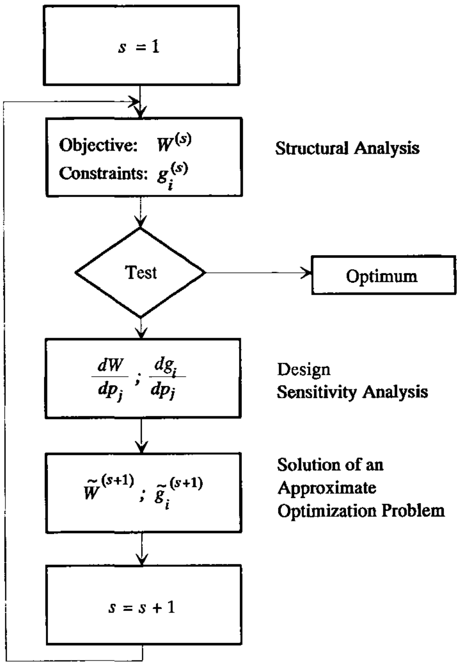

FIGURE 1 Optimization scheme.

tions of the objective function and constraints. The equality constraints of Eq. (4) are eliminated. The results of the sensitivity analysis are used to formulate this optimization problem, which can be solved by mathematical programming methods. Many algorithms have proven to be efficient for this purpose.

To illustrate the formulation of the approximate optimization problem, the method of convex linearization will be given here in a form similar to that used by Braibant and Fleury (1985). Using the sensitivity information in each iteration step, the objective function and the constraints are approximately

$$\tilde{f}^{(s+1)} = f(\mathbf{p}^{(s)}) + \sum_{j=1}^{n_p} (p_j - p_j^{(s)}) c_j \frac{d}{dp_j} f(\mathbf{p}^{(s)}). \quad (9)$$

The value of c_j is determined such that Eq. (9) is either a series expansion with respect to the design variables or their reciprocals and that the function $\tilde{f}^{(s+1)}$ assumes its largest value, i.e., the approximation is conservative. If all design variables are chosen to have positive values,

$$\begin{aligned} c_j &= 1 \quad \forall \frac{d}{dp_j} f(\mathbf{p}^{(s)}) > 0, \\ c_j &= \frac{p_j^{(s)}}{p_j} \quad \forall \frac{d}{dp_j} f(\mathbf{p}^{(s)}) < 0. \end{aligned} \quad (10)$$

Application of Eq. (9) to the structural optimization problem of Eq. (1) leads to the convex separable optimization problem

$$\begin{aligned} \tilde{W}^{(s+1)} &= \sum_{(dW/dp_j)>0} \frac{dW}{dp_j} p_j \\ &\quad - \sum_{(dW/dp_j)<0} \frac{dW}{dp_j} \frac{p_j^{(s)2}}{p_j} \Rightarrow \min, \\ \tilde{g}_i^{(s+1)} &= g_i^{(s)} + \sum_{(dg_i/dp_j)>0} \frac{dg_i}{dp_j} p_j \\ &\quad - \sum_{(dg_i/dp_j)<0} \frac{dg_i}{dp_j} \frac{p_j^{(s)2}}{p_j} - \sum_j \left| \frac{dg_i}{dp_j} \right| p_j^{(s)} \le 0. \end{aligned} \quad (11)$$

Methods of mathematical programming can be used to solve this optimization problem.

Sequential solutions for such approximate optimization problems leads ultimately to a solution for the structural optimization problem of Eq. (1). The optimization iteration over s stops if

$$|(W^{(s)} - W^{(s-1)})/W^{(s-1)}| < \varepsilon_W, \quad g_i^{(s)} < \varepsilon_g, \quad (12)$$

where ε_W and ε_g are predetermined tolerance values. The design optimization process using local function approximations determines local minima only. This is caused by the nature of the structural optimization problem. The structural optimization problem of Eq. (1) in general has no special characteristics such as convexity. If the problem would be convex the minimum could be characterized as a global minimum.

SENSITIVITY ANALYSIS FOR TRANSIENT RESPONSE

Design sensitivity analysis provides the gradient of the structural behavior with respect to the design variables p_j, $j = 1, \ldots, n_p$. The derivatives of the response functions with respect to the design variables will be called *design derivatives*. Design sensitivity analysis can be based on the continuum and on the discretized structure. Here, the latter will be applied. The differences between these approaches have been discussed widely in the literature. See, for example, Haug et al. (1986) and Arora (1995).

For the derivation of the design sensitivity coefficients from the discretized model of the structure, express the equation of motion of the structural system in the first-order form

$$\mathbf{P}\dot{\mathbf{u}} = \mathbf{f}(\mathbf{u}, \mathbf{p}, t), \quad \mathbf{u}(0) = \mathbf{u}_0. \tag{13}$$

This form can include both linear and nonlinear structural behavior (Hsieh and Arora, 1984). The state vector **u** contains the generalized velocities and displacements. The load vector **f** includes external and internal loads. Choose the response function g_i, $i = 1, \ldots, n_c = n_k + n_l$, written in the integral form

$$g_i = \int_0^{t_e} \psi_i(\dot{\mathbf{u}}, \mathbf{u}, \mathbf{p}, t)dt. \tag{14}$$

This derivation of a design sensitivity analysis follows the commonly used methodology, such as in Hsieh and Arora (1984), except that here the dependence of the response function on the vector $\dot{\mathbf{u}}$ is included. It is restricted to the case for which the design derivatives exist.

The simplest, but most expensive method to obtain design sensitivity information is to utilize *finite differences*. In this case the design variables are changed one at the time, with the design derivatives computed using

$$\frac{dg_i}{dp_j} = \frac{g_i(p_j + \Delta p_j) - g_i(p_j - \Delta p_j)}{2\Delta p_j}. \tag{15}$$

The parameter change Δp_j must be small enough to obtain accurate sensitivity information, but not too small because then numerical difficulties can occur. Here, central differences are given. Forward or backward differences can be erroneous. In the case of shape design variables, for example, the use of forward differences would cause a loss of design symmetries. Haftka (1981) shows that in some cases, for transient problems using explicit solution schemes, finite differences might be superior to the direct differentiation method of sensitivity analysis. The description of the direct differentiation method follows.

To develop analytical expressions for design sensitivity analysis, start with the derivatives of the response function of Eq. (14) with respect to the design variables p_j that follow as

$$\frac{dg_i}{dp_j} = \int_0^{t_e} \left(\frac{\partial\psi_i}{\partial p_j} + \frac{\partial\psi_i}{\partial \mathbf{u}}\frac{d\mathbf{u}}{dp_j} + \frac{\partial\psi_i}{\partial \dot{\mathbf{u}}}\frac{\dot{\mathbf{u}}}{dp_j}\right)dt. \tag{16}$$

The calculation of these derivatives requires knowledge of the design derivatives of the state variables. These can be obtained by differentiating Eq. (13) with respect to the design variables. Then,

$$\mathbf{P}\frac{d\dot{\mathbf{u}}}{dp_j} - \frac{\partial \mathbf{f}}{\partial \mathbf{u}}\frac{d\mathbf{u}}{dp_j} = \mathbf{q}, \quad \frac{d\mathbf{u}(0)}{dp_j} = \mathbf{0}, \tag{17}$$

with

$$\mathbf{q} = \frac{\partial \mathbf{f}}{\partial p_j} - \frac{\partial \mathbf{P}}{\partial p_j}\dot{\mathbf{u}}. \tag{18}$$

The solution of Eq. (17) determines the design derivatives of the state variables. This method of sensitivity analysis is called the *direct differentiation method*. For each design variable the system equation, Eq. (17), has to be solved. This can be quite expensive if the number of design variables is large.

If the number of response functions that are needed for the solution of the optimization problem is smaller than the number of design variables, an *adjoint variable method* should be used for sensitivity analysis. Begin by rearranging the design derivatives of the response function of Eq. (16), in which $d\dot{\mathbf{u}}/dp_j$ is replaced by the first relation of Eq. (17). Then,

$$\frac{dg_i}{dp_j} = \int_0^{t_e} \left[\frac{\partial\psi_i}{\partial p_j} + \left(\frac{\partial\psi_i}{\partial \mathbf{u}} + \frac{\partial\psi_i}{\partial \dot{\mathbf{u}}}\mathbf{P}^{-1}\frac{\partial \mathbf{f}}{\partial \mathbf{u}}\right)\frac{d\mathbf{u}}{dp_j} + \frac{\partial\psi_i}{\partial \dot{\mathbf{u}}}\mathbf{P}^{-1}\mathbf{q}\right]dt. \tag{19}$$

Multiplication of Eq. (17) with the adjoint variable $\mathbf{a}^T$, and integration over time leads to

$$\int_0^{t_e} \mathbf{a}^T\left(\mathbf{P}\frac{d\dot{\mathbf{u}}}{dp_j} - \frac{\partial \mathbf{f}}{\partial \mathbf{u}}\frac{d\mathbf{u}}{dp_j}\right)dt = \int_0^{t_e} \mathbf{a}^T\mathbf{q}dt. \tag{20}$$

Integration by parts provides

$$\mathbf{a}^T\mathbf{P}\frac{d\mathbf{u}}{dp_j}\bigg|_0^{t_e} - \int_0^{t_e}\left(\dot{\mathbf{a}}^T\mathbf{P} + \mathbf{a}^T\dot{\mathbf{P}} + \mathbf{a}^T\frac{\partial \mathbf{f}}{\partial \mathbf{u}}\right)\frac{d\mathbf{u}}{dp_j}dt = \int_0^{t_e}\mathbf{a}^T\mathbf{q}dt. \tag{21}$$

The first term on the left-hand side vanishes due to the initial condition of Eq. (17) and if the terminal condition $\mathbf{a}(t_e) = \mathbf{0}$ is introduced. By comparison of Eqs. (21) and (19), the second term of Eq. (19) can be found as

$$\int_0^{t_e}\left(\frac{\partial\psi_i}{\partial \mathbf{u}} + \frac{\partial\psi_i}{\partial \dot{\mathbf{u}}}\mathbf{P}^{-1}\frac{\partial \mathbf{f}}{\partial \mathbf{u}}\right)\frac{d\mathbf{u}}{dp_j}dt = -\int_0^{t_e}\mathbf{a}^T\mathbf{q}dt, \tag{22}$$

where **a** is subject to the adjoint equation

$$\mathbf{P}^T\dot{\mathbf{a}} + \left(\dot{\mathbf{P}} + \frac{\partial \mathbf{f}}{\partial \mathbf{u}}\right)^T \mathbf{a} = \left(\frac{\partial \psi_i}{\partial \mathbf{u}} + \frac{\partial \psi_i}{\partial \dot{\mathbf{u}}}\mathbf{P}^{-1}\frac{\partial \mathbf{f}}{\partial \mathbf{u}}\right)^T, \quad \mathbf{a}(t_e) = \mathbf{0}. \tag{23}$$

This is a linear equation that has to be integrated backward to meet the terminal condition. Finally, Eq. (16) can be rewritten. Using Eq. (23) and **q** of Eq. (18),

$$\frac{dg_i}{dp_j} = \int_0^{t_e}\left[\frac{\partial \psi_i}{\partial p_j} - \left(\mathbf{a}^T - \frac{\partial \psi_i}{\partial \dot{\mathbf{u}}}\mathbf{P}^{-1}\right)\mathbf{q}\right]dt. \tag{24}$$

In the case that the constraint g_i is a pointwise constraint, the adjoint equation can be simplified (Haftka et al., 1990). Equation (23) then becomes

$$\mathbf{P}^T\dot{\mathbf{a}} + \left(\dot{\mathbf{P}} + \frac{\partial \mathbf{f}}{\partial \mathbf{u}}\right)^T \mathbf{a} = \left(\frac{\partial \psi_i}{\partial \mathbf{u}} + \frac{\partial \psi_i}{\partial \dot{\mathbf{u}}}\mathbf{P}^{-1}\frac{\partial \mathbf{f}}{\partial \mathbf{u}}\right)^T \delta(t - t_c), \quad \mathbf{a}(t_e) = \mathbf{0}. \tag{25}$$

Integration from $t_c - \varepsilon$ to $t_c + \varepsilon$ leads to

$$\mathbf{P}^T\dot{\mathbf{a}} + \left(\dot{\mathbf{P}} + \frac{\partial \mathbf{f}}{\partial \mathbf{u}}\right)^T \mathbf{a} = \mathbf{0}, \quad \mathbf{a}(t_c) = -\left(\frac{\partial \psi_i(t_c)}{\partial \mathbf{u}} + \frac{\partial \psi_i(t_c)}{\partial \dot{\mathbf{u}}}\mathbf{P}^{-1}\frac{\partial \mathbf{f}(t_c)}{\partial \mathbf{u}}\right)\mathbf{P}^{-1}. \tag{26}$$

These formulas for sensitivity analysis can be used for structural discretizations that consist of springs, masses, and dampers as well as for systems discretized using finite elements. The type of discretization has an influence on the computation of the design derivatives of the structural matrices, i.e., $\partial\mathbf{P}/\partial p_j$, $\partial\mathbf{f}/\partial p_j$, $\partial\mathbf{f}/\partial\mathbf{u}$. Two concepts are possible. First, the analytical method, where these derivatives are computed from the formulation of the matrices. Second, the semianalytical method, where the derivatives $\partial\mathbf{P}/\partial p_j$, $\partial\mathbf{f}/\partial p_j$ fully or in part are calculated using finite differences. The decision as to which to use should be made depending on the effort for the implementation.

Rigid body systems are often used for concept models, for example, in automobile design. Optimization here can help in an early design stage to make the appropriate decision that influences the behavior of the final design. Continuum models discretized using finite elements can be employed for design improvements in a later stage of the design process.

NONLINEAR DYNAMIC STRUCTURES

The methodology for a sensitivity analysis described above will now be applied to nonlinear dynamic structures. Finite elements are used to derive the state equation. Here, the methodology presented in the text by Bathe (1995) will be adopted as the solution technique for the nonlinear dynamic problem.

Figure 2 shows a structure of volume ${}^0\Omega$. Tractions ${}^t\mathbf{t}$ are defined on the boundary ${}^0\Gamma_\sigma$, and displacements ${}^t\mathbf{v}_0$ are defined on the boundary ${}^0\Gamma_u$. For nonlinear computations two incremental formulations are practicable. One is the total Lagrangian formulation where all static and kinematic variables refer to the configuration at time $t = 0$, and the other is the updated Lagrangian formulation where the variables refer to the configuration of the previous time step (Bathe, 1995). The total Lagrangian formulation will be utilized here. Then, the principle of virtual work is given as

$$\int_{{}^0\Omega} {}^0\rho\, {}^t\ddot{\mathbf{v}}^T \delta\mathbf{v}\, d{}^0\Omega + \int_{{}^0\Omega} {}^t\mathbf{s}^T \delta {}^t\mathbf{e}\, d{}^0\Omega = \int_{{}^0\Omega} {}^t\mathbf{b}^T \delta\mathbf{v}\, d{}^0\Omega + \int_{{}^0\Gamma} {}^t\mathbf{t}^T \delta\mathbf{v}\, d{}^0\Gamma. \tag{27}$$

In this equation, ${}^t\mathbf{s}$ is the vector of second Piola–Kirchhoff stresses, the vector $\delta{}^t\mathbf{e}$ contains the variations in the Green–Lagrange strains, and ${}^t\mathbf{b}$ is the vector of body forces. Depending on the solution scheme, finite element equations for explicit and implicit time integration can be established. The presentation here will be restricted to

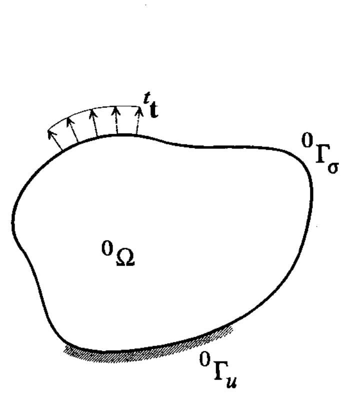

FIGURE 2 Structure.

the explicit integration schemes. Introduce the approximation

$$ {}^t\mathbf{v} = \mathbf{N}\,{}^t\mathbf{d} \qquad (28) $$

into the principle of Eq. (27). This leads to the system equation for explicit time integration

$$ \mathbf{M}\,{}^t\ddot{\mathbf{d}} = {}^t\mathbf{f}_{\text{ext}} - {}^t\mathbf{f}_{\text{int}}, \quad {}^0\mathbf{d} = \mathbf{d}_0, \quad {}^0\dot{\mathbf{d}} = \dot{\mathbf{d}}_0. \qquad (29) $$

The time independent mass matrix $\mathbf{M}$ follows from the element mass matrices $\mathbf{M}^e$ that appear as

$$ \mathbf{M}^e = \int_{{}^0\Omega} {}^0\rho \mathbf{N}^T \mathbf{N}\, d\,{}^0\Omega. \qquad (30) $$

The internal load vector ${}^t\mathbf{f}_{\text{int}}$ is calculated from

$$ {}^t\mathbf{f}^e_{\text{int}} = \int_{{}^0\Omega} {}^t\mathbf{B}_L^T\, {}^t\mathbf{s}\, d\,{}^0\Omega, \qquad (31) $$

using the vector of second Piola–Kirchhoff stresses ${}^t\mathbf{s}$. The quantity ${}^t\mathbf{B}_L$ is the linear strain-displacement matrix. The external loads are assembled in the vector ${}^t\mathbf{f}_{\text{ext}}$. A solution scheme for Eq. (29) using central differences is given in the Appendix.

A sensitivity analysis using the explicit integration scheme of Eq. (29) can be derived. The derivatives of the functional g_i of Eq. (14) with respect to the design variable p_j appear as

$$ \frac{dg_i}{dp_j} = \int_0^{t_e} \left(\frac{\partial^t\psi_i}{\partial p_j} + \frac{\partial^t\psi_i}{\partial \mathbf{d}} \frac{d^t\mathbf{d}}{dp_j} + \frac{\partial^t\psi_i}{\partial \dot{\mathbf{d}}} \frac{d^t\dot{\mathbf{d}}}{dp_j} + \frac{\partial^t\psi_i}{\partial \ddot{\mathbf{d}}} \frac{d^t\ddot{\mathbf{d}}}{dp_j} \right) dt. \qquad (32) $$

Using direct differentiation, the derivatives of the displacement vector with respect to the design variables can be obtained from

$$ \mathbf{M} \frac{d^t\ddot{\mathbf{d}}}{dp_j} + \frac{\partial^t\mathbf{f}_{\text{int}}}{\partial \dot{\mathbf{d}}} \frac{d^t\dot{\mathbf{d}}}{dp_j} + \frac{\partial^t\mathbf{f}_{\text{int}}}{\partial \mathbf{d}} \frac{d^t\mathbf{d}}{dp_j} = {}^t\overline{\mathbf{q}}, \qquad \frac{d^0\mathbf{d}}{dp_j} = 0, \quad \frac{d^0\dot{\mathbf{d}}}{dp_j} = 0, \qquad (33) $$

with

$$ {}^t\overline{\mathbf{q}} = -\left(\frac{\partial^t\mathbf{f}_{\text{int}}}{\partial p_j} + \frac{\partial \mathbf{M}}{\partial p_j}\, {}^t\ddot{\mathbf{d}} \right). \qquad (34) $$

The solution scheme for Eq. (33) is given in the Appendix.

To derive an adjoint variable method, start with the substitution of $d^t\ddot{\mathbf{d}}/dp_j$ in Eq. (32) using Eq. (33). Then,

$$ \frac{dg_i}{dp_j} = \int_0^{t_e} \frac{\partial^t\psi_i}{\partial p_j} dt + \int_0^{t_e} \frac{\partial^t\psi_i}{\partial \ddot{\mathbf{d}}} \mathbf{M}^{-1} \overline{\mathbf{q}} dt + \int_0^{t_e} \left(\frac{\partial^t\psi_i}{\partial \mathbf{d}} - \frac{\partial^t\psi_i}{\partial \ddot{\mathbf{d}}} \mathbf{M}^{-1} \frac{\partial^t\mathbf{f}_{\text{int}}}{\partial \mathbf{d}} \right) \frac{d^t\mathbf{d}}{dp_j} dt + \int_0^{t_e} \left(\frac{\partial^t\psi_i}{\partial \dot{\mathbf{d}}} - \frac{\partial^t\psi_i}{\partial \ddot{\mathbf{d}}} \mathbf{M}^{-1} \frac{\partial^t\mathbf{f}_{\text{int}}}{\partial \dot{\mathbf{d}}} \right) \frac{d^t\dot{\mathbf{d}}}{dp_j} dt. \qquad (35) $$

For the final two integrals on the right-hand side, adjoint equations are to be found. Again, multiply the design derivative of the state equation of Eq. (33) with the adjoint variable ${}^t\mathbf{a}^T$

$$ \int_0^{t_e} {}^t\mathbf{a}^T \left(\mathbf{M} \frac{d^t\ddot{\mathbf{d}}}{dp_j} + \frac{\partial^t\mathbf{f}_{\text{int}}}{\partial \dot{\mathbf{d}}} \frac{d^t\dot{\mathbf{d}}}{dp_j} + \frac{\partial^t\mathbf{f}_{\text{int}}}{\partial \mathbf{d}} \frac{d^t\mathbf{d}}{dp_j} \right) dt = \int_0^{t_e} {}^t\mathbf{a}^T\, {}^t\overline{\mathbf{q}} dt. \qquad (36) $$

Integration by parts yields

$$ {}^t\mathbf{a}^T \mathbf{M} \frac{d^t\dot{\mathbf{d}}}{dp_j}\bigg|_0^{t_e} + \int_0^{t_e} \left(-{}^t\dot{\mathbf{a}}^T \mathbf{M} + {}^t\mathbf{a}^T \frac{\partial^t\mathbf{f}_{\text{int}}}{\partial \dot{\mathbf{d}}} \right) \frac{d^t\dot{\mathbf{d}}}{dp_j} dt + \int_0^{t_e} {}^t\mathbf{a}^T \frac{\partial^t\mathbf{f}_{\text{int}}}{\partial \mathbf{d}} \frac{d^t\mathbf{d}}{dp_j} dt = \int_0^{t_e} {}^t\mathbf{a}^T\, {}^t\overline{\mathbf{q}} dt, \qquad (37) $$

and a second integration by parts leads to

$$ {}^t\mathbf{a}^T \mathbf{M} \frac{d^t\dot{\mathbf{d}}}{dp_j}\bigg|_0^{t_e} - {}^t\dot{\mathbf{a}}^T \mathbf{M} \frac{d\mathbf{d}}{dp_j}\bigg|_0^{t_e} + {}^t\mathbf{a}^T \frac{\partial^t\mathbf{f}_{\text{int}}}{\partial \dot{\mathbf{d}}} \frac{d\mathbf{d}}{dp_j}\bigg|_0^{t_e} + \int_0^{t_e} \left({}^t\ddot{\mathbf{a}}^T \mathbf{M} - {}^t\dot{\mathbf{a}}^T \frac{\partial^t\mathbf{f}_{\text{int}}}{\partial \dot{\mathbf{d}}} \right) + {}^t\mathbf{a}^T \frac{\partial^t\mathbf{f}_{\text{int}}}{\partial \mathbf{d}} \Big) \frac{d^t\mathbf{d}}{dp_j} dt = \int_0^{t_e} {}^t\mathbf{a}^T\, {}^t\overline{\mathbf{q}} dt. \qquad (38) $$

It is assumed that the term $\partial^t\mathbf{f}_{\text{int}}/\partial\dot{\mathbf{d}}$ is time independent. The first three terms vanish if the terminal conditions ${}^{t_e}\mathbf{a} = 0$, ${}^{t_e}\dot{\mathbf{a}} = 0$ are satisfied.

To determine the third integral of Eq. (35), solve the adjoint equation that follows from Eq. (38)

$$\mathbf{M}{}^t\ddot{\mathbf{a}}_1 - \frac{\partial^t\mathbf{f}_{\text{int}}}{\partial\dot{\mathbf{d}}}{}^t\dot{\mathbf{a}}_1 + \frac{\partial^t\mathbf{f}_{\text{int}}}{\partial\mathbf{d}}{}^t\mathbf{a}_1 = \left(\frac{\partial^t\psi_i}{\partial\mathbf{d}} - \frac{\partial^t\psi_i}{\partial\ddot{\mathbf{d}}}\mathbf{M}^{-1}\frac{\partial^t\mathbf{f}_{\text{int}}}{\partial\mathbf{d}}\right)^T, \quad {}^{t_e}\mathbf{a}_1 = 0, \quad {}^{t_e}\dot{\mathbf{a}}_1 = 0. \tag{39}$$

This yields

$$\int_0^{t_e}\left(\frac{\partial^t\psi_i}{\partial\mathbf{d}} - \frac{\partial^t\psi_i}{\partial\ddot{\mathbf{d}}}\mathbf{M}^{-1}\frac{\partial^t\mathbf{f}_{\text{int}}}{\partial\mathbf{d}}\right)\frac{d^t\mathbf{d}}{dp_j}\,dt = \int_0^{t_e}{}^t\mathbf{a}_1^T\,{}^t\bar{\mathbf{q}}dt. \tag{40}$$

For the fourth integral of Eq. (35), two adjoint equations are introduced. From the first integral of Eq. (37) follows

$$-\mathbf{M}{}^t\dot{\mathbf{a}}_2 + \frac{\partial^t\mathbf{f}_{\text{int}}}{\partial\dot{\mathbf{d}}}{}^t\mathbf{a}_2 = \left(\frac{\partial^t\psi_i}{\partial\dot{\mathbf{d}}} - \frac{\partial^t\psi_i}{\partial\ddot{\mathbf{d}}}\mathbf{M}^{-1}\frac{\partial^t\mathbf{f}_{\text{int}}}{\partial\dot{\mathbf{d}}}\right)^T, \quad {}^{t_e}\mathbf{a}_2 = 0, \tag{41}$$

that leads to

$$\int_0^{t_e}\left(\frac{\partial^t\psi_i}{\partial\dot{\mathbf{d}}} - \frac{\partial^t\psi_i}{\partial\ddot{\mathbf{d}}}\mathbf{M}^{-1}\frac{\partial^t\mathbf{f}_{\text{int}}}{\partial\dot{\mathbf{d}}}\right)\frac{d^t\dot{\mathbf{d}}}{dp_j}\,dt = \int_0^{t_e}{}^t\mathbf{a}_2^T\,{}^t\bar{\mathbf{q}}dt - \int_0^{t_e}{}^t\mathbf{a}_2^T\frac{\partial^t\mathbf{f}_{\text{int}}}{\partial\mathbf{d}}\frac{d^t\mathbf{d}}{dp_j}\,dt. \tag{42}$$

This would leave the second integral on the right-hand side that can be determined by a third adjoint equation that follows from Eq. (38)

$$\mathbf{M}{}^t\ddot{\mathbf{a}}_3 - \frac{\partial^t\mathbf{f}_{\text{int}}}{\partial\dot{\mathbf{d}}}{}^t\dot{\mathbf{a}}_3 + \frac{\partial^t\mathbf{f}_{\text{int}}}{\partial\mathbf{d}}{}^t\mathbf{a}_3 = -\frac{\partial^t\mathbf{f}_{\text{int}}}{\partial\mathbf{d}}{}^t\mathbf{a}_2, \quad {}^{t_e}\mathbf{a}_3 = 0, \quad {}^{t_e}\dot{\mathbf{a}}_3 = 0. \tag{43}$$

Then,

$$\int_0^{t_e}\left(\frac{\partial^t\psi_i}{\partial\dot{\mathbf{d}}} - \frac{\partial^t\psi_i}{\partial\ddot{\mathbf{d}}}\mathbf{M}^{-1}\frac{\partial^t\mathbf{f}_{\text{int}}}{\partial\dot{\mathbf{d}}}\right)\frac{d^t\dot{\mathbf{d}}}{dp_j}\,dt = \int_0^{t_e}({}^t\mathbf{a}_2 + {}^t\mathbf{a}_3)^T\,{}^t\bar{\mathbf{q}}dt. \tag{44}$$

For higher computational efficiency, the adjoint equations, Eqs. (39) and (43), can be solved simultaneously considering the fact that both are linear equations. This leads to the system equation

$$\mathbf{M}{}^t\ddot{\mathbf{a}}_4 - \frac{\partial^t\mathbf{f}_{\text{int}}}{\partial\dot{\mathbf{d}}}{}^t\dot{\mathbf{a}}_4 + \frac{\partial^t\mathbf{f}_{\text{int}}}{\partial\mathbf{d}}{}^t\mathbf{a}_4 = \left[\frac{\partial^t\psi_i}{\partial\mathbf{d}} - \left(\frac{\partial^t\psi_i}{\partial\ddot{\mathbf{d}}}\mathbf{M}^{-1} + {}^t\mathbf{a}_2^T\right)\frac{\partial^t\mathbf{f}_{\text{int}}}{\partial\mathbf{d}}\right]^T, \quad {}^{t_e}\mathbf{a}_4 = 0, \quad {}^{t_e}\dot{\mathbf{a}}_4 = 0. \tag{45}$$

Finally, the design derivatives of the response function appear as

$$\frac{dg_i}{dp_j} = \int_0^{t_e}\left[\frac{\partial^t\psi_i}{\partial p_j} + \left({}^t\mathbf{a}_2^T + {}^t\mathbf{a}_2^T + \frac{\partial^t\psi_i}{\partial\ddot{\mathbf{d}}}\mathbf{M}^{-1}\right){}^t\bar{\mathbf{q}}\right]dt, \tag{46}$$

where ${}^t\mathbf{a}_2$, ${}^t\mathbf{a}_4$ are subject to the adjoint equations, Eqs. (41) and (45), respectively. These adjoint equations have to be integrated backward to meet the terminal conditions. A central differences solution scheme is provided in the Appendix.

To complete the sensitivity analysis, the design derivatives of the element mass matrix and of the element internal load vector have to be found. These can be determined by applying the chain rule. From Eq. (30) follows

$$\frac{\partial\mathbf{M}^e}{\partial p_j} = \int_{{}^0\Omega}{}^0\rho\nabla^T(\mathbf{N}^T\mathbf{N}\mathbf{V}({}^0\mathbf{x}))d^0\Omega. \tag{47}$$

For the internal load vector ${}^t\mathbf{f}_{\text{int}}$, from Eq. (31),

$$\frac{\partial^t\mathbf{f}_{\text{int}}^e}{\partial p_j} = \int_{{}^0\Omega}\left[\frac{\partial^t\mathbf{B}_L^T}{\partial p_j}{}^t\mathbf{s} + {}^t\mathbf{B}_L^T\frac{\partial^t\mathbf{s}}{\partial p_j} + \nabla^T({}^t\mathbf{B}_L^T\,{}^t\mathbf{s}\mathbf{V}({}^0\mathbf{x}))\right]d^0\Omega. \tag{48}$$

The vector ∇ is the nabla operator. The design velocity field $\mathbf{V}({}^0\mathbf{x})$ represents the derivatives of the position vector of a point of the structure with respect to the design variables (Fig. 3), such that

$${}^0\mathbf{x}^{(s+1)} = {}^0\mathbf{x}^{(s)} + \mathbf{V}({}^0\mathbf{x})\delta^0\mathbf{x}, \tag{49}$$

where $\delta^0\mathbf{x}$ is the variation of the position ${}^0\mathbf{x}$. Several methods for the computation of the design velocity field for shape optimization are available (Chang and Choi, 1992; Schramm and Pilkey, 1993). In each optimization step the design velocity field has to be found only for the initial configuration.

The computation of the matrices of Eqs. (47) and (48) depends much on the type of structural optimization problem at hand. For sizing optimi-

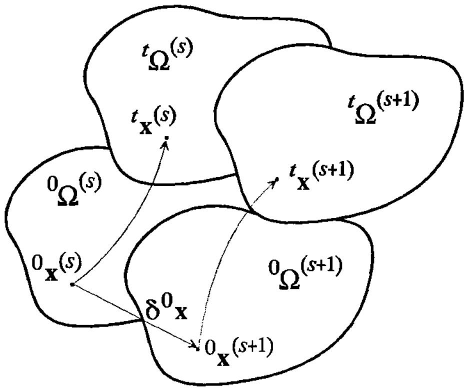

FIGURE 3 Design configurations.

zation problems these derivatives can be simplified, because the sizing variables such as cross-sectional properties of beams or plate thicknesses often appear as a factor in front of the integral. For shape optimization problems and for problems that involve material properties, the computation of Eqs. (47) and (48) is much more complicated.

CONCLUDING REMARKS

The optimization of structures under impact loading is a relatively young subject in structural optimization research. Certainly there is potential for new developments in this field, especially for complex structures. Optimization methods can help to speed up design decisions. Expensive parameter studies can be eliminated if design sensitivity information becomes available. But numerical optimization tools are only one ingredient to determine the layout of structural designs. The design engineer still must weigh the results to draw conclusions for design changes. The impact behavior of the structure is only one area of the complexity of the structural behavior. The whole design process is a multidisciplinary task where the creativity of the designer plays the major role.

APPENDIX: SOLUTION SCHEMES

This Appendix provides a description of the central differences procedure for the solution of the system equations in the text.

1. Solution of the state equation, Eq. (29) Bathe, 1995):

$$\frac{1}{\Delta t^2}\mathbf{M}^{t+\Delta t}\mathbf{d} = {}^t\mathbf{f}_{\text{ext}} - {}^t\mathbf{f}_{\text{int}}\ \frac{1}{\Delta t^2}\mathbf{M}({}^{t-\Delta t}\mathbf{d} - 2{}^t\mathbf{d}). \tag{A.1}$$

Initialization:

$$\begin{aligned} {}^0\mathbf{d} &= \mathbf{d}_0, \quad {}^0\dot{\mathbf{d}} = \dot{\mathbf{d}}_0, \\ {}^0\ddot{\mathbf{d}} &= \mathbf{M}^{-1}({}^0\mathbf{f}_{\text{ext}} - {}^0\mathbf{f}_{\text{int}}), \\ {}^{-\Delta t}\mathbf{d} &= {}^0\mathbf{d} - \Delta t\,{}^0\dot{\mathbf{d}} + \frac{\Delta t^2}{2}\,{}^0\ddot{\mathbf{d}}. \end{aligned} \tag{A.2}$$

Velocities:

$${}^t\dot{\mathbf{d}} = \frac{1}{2\Delta t}(-{}^{t-\Delta t}\mathbf{d} + {}^{t+\Delta t}\mathbf{d}). \tag{A.3}$$

Accelerations:

$${}^t\ddot{\mathbf{d}} = \frac{1}{\Delta t^2}({}^{t-\Delta t}\mathbf{d} - 2{}^t\mathbf{d} + {}^{t+\Delta t}\mathbf{d}). \tag{A.4}$$

2. Solution of Eq. (33):

$$\begin{aligned} \left(\frac{1}{\Delta t^2}\mathbf{M} + \frac{1}{2\Delta t}\frac{\partial{}^t\mathbf{f}_{\text{int}}}{\partial\dot{\mathbf{d}}}\right)\frac{d^{t+\Delta t}\mathbf{d}}{dp_j} &= -\left(\frac{\partial\mathbf{M}}{\partial p_j}{}^t\ddot{\mathbf{d}} + \frac{\partial{}^t\mathbf{f}_{\text{int}}}{\partial p_j}\right) \\ &\quad + \left(\frac{2}{\Delta t^2}\mathbf{M} - \frac{\partial{}^t\mathbf{f}_{\text{int}}}{\partial\mathbf{d}}\right)\frac{d^t\mathbf{d}}{dp_j} \\ &\quad - \left(\frac{1}{\Delta t^2}\mathbf{M} - \frac{1}{2\Delta t}\frac{\partial{}^t\mathbf{f}_{\text{int}}}{\partial\dot{\mathbf{d}}}\right)\frac{d^{t-\Delta t}\mathbf{d}}{dp_j}. \end{aligned} \tag{A.5}$$

Initialization:

$$\begin{aligned} &\frac{d^0\mathbf{d}}{dp_j} = \mathbf{0}, \quad \frac{d^0\dot{\mathbf{d}}}{dp_j} = \mathbf{0}, \\ &\frac{d^0\ddot{\mathbf{d}}}{dp_j} = -\mathbf{M}^{-1}\left(\frac{\partial\mathbf{M}}{\partial p_j}{}^0\ddot{\mathbf{d}} + \frac{\partial^0\mathbf{f}_{\text{int}}}{\partial p_j}\right), \\ &\frac{d^{-\Delta t}\mathbf{d}}{dp_j} = \frac{\Delta t^2}{2}\frac{d^0\ddot{\mathbf{d}}}{dp_j}. \end{aligned} \tag{A.6}$$

Design derivatives of the velocities:

$$\frac{d^t\dot{\mathbf{d}}}{dp_j} = \frac{1}{2\Delta t}\left(-\frac{d^{t-\Delta t}\mathbf{d}}{dp_j} + \frac{d^{t+\Delta t}\mathbf{d}}{dp_j}\right). \tag{A.7}$$

Design derivatives of the accelerations:

$$\frac{d^t\ddot{\mathbf{d}}}{dp_j} = \frac{1}{\Delta t^2}\left(\frac{d^{t-\Delta t}\mathbf{d}}{dp_j} - 2\,\frac{d^t\mathbf{d}}{dp_j} + \frac{d^{t+\Delta t}\mathbf{d}}{dp_j}\right). \tag{A.8}$$

3. Solution of the adjoint Eqs. (41) and (45):

$$\begin{aligned}\frac{1}{2\Delta t}\,\mathbf{M}^{t-\Delta t}\mathbf{a}_2 &= \left[\frac{\partial^t\psi_i}{\partial\dot{\mathbf{d}}} - \left(\frac{\partial^t\psi_i}{\partial\ddot{\mathbf{d}}}\,\mathbf{M}^{-1} + {}^t\mathbf{a}_2^T\right)\frac{\partial^t\mathbf{f}_{\text{int}}}{\partial\dot{\mathbf{d}}}\right]^T \\ &\quad + \frac{1}{2\Delta t}\,\mathbf{M}^{t+\Delta t}\mathbf{a}_2,\end{aligned} \tag{A.9}$$

$$\begin{aligned}\left(\frac{1}{\Delta t^2}\,\mathbf{M} + \frac{1}{2\Delta t}\,\frac{\partial^t\mathbf{f}_{\text{int}}}{\partial\dot{\mathbf{d}}}\right){}^{t-\Delta t}\mathbf{a}_4 &= \left[\frac{\partial^t\psi_i}{\partial\mathbf{d}} - \left(\frac{\partial^t\psi_i}{\partial\ddot{\mathbf{d}}}\,\mathbf{M}^{-1} + {}^t\mathbf{a}_2^T\right)\frac{\partial^t\mathbf{f}_{\text{int}}}{\partial\mathbf{d}}\right]^T \\ &\quad + \left(\frac{2}{\Delta t^2}\,\mathbf{M} - \frac{\partial^t\mathbf{f}_{\text{int}}}{\partial\mathbf{d}}\right){}^t\mathbf{a}_4 \\ &\quad - \left(\frac{1}{\Delta t^2}\,\mathbf{M} - \frac{1}{2\Delta t}\,\frac{\partial^t\mathbf{f}_{\text{int}}}{\partial\dot{\mathbf{d}}}\right){}^{t+\Delta t}\mathbf{a}_4.\end{aligned} \tag{A.10}$$

Initialization:

$$\begin{aligned}{}^{t_e}\mathbf{a}_2 &= \mathbf{0}, \\ {}^{t_e+\Delta t}\mathbf{a}_2 &= -\Delta t\mathbf{M}^{-1}\left(\frac{\partial^{t_e}\psi_i}{\partial\dot{\mathbf{d}}} - \frac{\partial^{t_e}\psi_i}{\partial\ddot{\mathbf{d}}}\,\mathbf{M}^{-1}\,\frac{\partial^{t_e}\mathbf{f}_{\text{int}}}{\partial\dot{\mathbf{d}}}\right)^T, \\ {}^{t_e}\mathbf{a}_4 &= \mathbf{0}, \\ {}^{t_e+\Delta t}\mathbf{a}_4 &= \frac{\Delta t^2}{2}\,\mathbf{M}^{-1}\left(\frac{\partial^{t_e}\psi_i}{\partial\mathbf{d}} - \frac{\partial^{t_e}\psi_i}{\partial\ddot{\mathbf{d}}}\,\mathbf{M}^{-1}\,\frac{\partial^{t_e}\mathbf{f}_{\text{int}}}{\partial\mathbf{d}}\right)^T\end{aligned} \tag{A.11}$$

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