

Tangent Operators and Design Sensitivity Formulations for Transient Nonlinear Coupled Problems with Applications to Elasto-Plasticity

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Abstract

Tangent operators and design sensitivities are derived for transient nonlinear coupled problems. The solution process and the formation of tangent operators are presented in a systematic manner and sensitivities for a generalized response function are formulated via both the direct differentiation and adjoint methods. The derived formulations are suitable for finite element implementations. Analyses of systems with materials that exhibit history dependent response, may be obtained directly by applying the analyses of transient nonlinear coupled systems. Rate-independent elasto-plasticity is investigated as a case study and a problem with an analytical solution is analyzed for demonstration purposes.

1 Introduction

Efficient and accurate design sensitivity formulations based on both the direct differentiation and the adjoint methods have been developed over the last fifteen years. These methods replace the traditional finite difference method which is prohibitively expensive for practical applications, particularly when the number of design parameters is large; additionally it may be inaccurate due to round-off or truncation errors [1, 2]. On the other hand, the computations associated with the explicit sensitivity methods require only a small fraction of the original analysis cost. Unfortunately, unlike the finite difference method which is straightforward to implement, these explicit methods usually require laborious derivations. Moreover, their formulations are dependent upon the class of the boundary-value problem being solved.

Analytic design sensitivity analysis formulations for linear systems are well established [3, 4, 5]. However, the development of analytic design sensitivity analysis formulations for nonlinear systems is an area of on-going research. Several works formulate sensitivity expressions for steady-state uncoupled nonlinear systems (cf. [6, 7, 8, 9, 10, 11, 12, 13, 14, 15]). Design sensitivity analyses for transient uncoupled systems are addressed in [2, 16, 17, 18, 19, 20, 21]. Sensitivity analyses for steady-state coupled systems appear in [22, 23], and sensitivity analyses for transient coupled systems are investigated in [24, 25, 26, 27, 28, 29, 30, 31, 32, 33, 34, 35].

Vidal and Haber [34] emphasize that accurate design sensitivities may be computed only when the design sensitivity formulation is fully consistent with the underlying simulation model. They also show, in the context of elasto-plastic systems, that this consistent sensitivity derivation necessitates the use of the algorithmic tangent operator [30, 36].

Here, we clearly show that the tangent operators appearing in the Newton-Raphson solution of nonlinear systems are required for accurate design sensitivity analyses of transient coupled nonlinear problems. Sensitivities for steady-state and transient uncoupled nonlinear problems are initially presented. Then, the formulations are extended to steady-state and transient coupled nonlinear systems. These sensitivity expressions are formulated by both the direct differentiation and adjoint methods. Analyses of systems that exhibit history-dependent material response, e.g. plasticity, may be obtained directly by applying the analyses of transient nonlinear coupled systems. The direct differentiation results are consistent with the derivations in [30, 34]. The adjoint results are uniquely applied to the plasticity problem and are consistent with adjoint derivations for other coupled problems, e.g. thermo-elasticity [27, 31].

A systematic numerical approach to compute the algorithmic tangent operator is described. This approach is consistent with that of [37] and is a numerical alternative to the closed-form approach presented in [36], and may prove advantageous as it is compact and flexible, especially when complex constitutive relations are used. Furthermore, our approach facilitates a systematic modular computer implementation.

We demonstrate the versatility of our general formulation by particularizing it to rate-independent elasto-plasticity. A simple one-dimensional example with an analytical solution is presented where the sensitivities are evaluated by the both direct differentiation and adjoint methods.

2 General Formulation

In this section, we formulate a general approach for the primal¹ analysis and the subsequent sensitivity analysis for transient nonlinear coupled problems. The primal problem is expressed in residual form and solved iteratively by the Newton-Raphson method. Then, the sensitivities are derived. Steady-state uncoupled nonlinear problems are initially studied; gradually, the formulation is extended to accommodate transient coupled nonlinear problems. For transient systems, the time domain is discretized. Both the direct differentiation and adjoint approaches are explored. In all cases, the sensitivities are evaluated for a generalized response functional.

2.1 Steady-State Nonlinear Systems

A steady-state nonlinear problem may be expressed in residual form as

$$\mathbf{R}(\mathbf{u}) = \mathbf{0} \quad (1)$$

where \mathbf{R} is the residual and \mathbf{u} is the unknown system response. Equation (1) is solved iteratively by invoking the Newton-Raphson method. If the current iterate \mathbf{u}^I is not a solution, i.e. if $\mathbf{R}(\mathbf{u}^I) \neq \mathbf{0}$, then the next iterate \mathbf{u}^{I+1} is computed by equating the first-order Taylor series expansion of \mathbf{R} about \mathbf{u}^I to zero, i.e.

$$\mathbf{R}(\mathbf{u}^{I+1}) = \mathbf{R}(\mathbf{u}^I + \delta\mathbf{u}) \approx \mathbf{R}(\mathbf{u}^I) + \frac{D\mathbf{R}}{D\mathbf{u}}(\mathbf{u}^I)\delta\mathbf{u} = \mathbf{0} \quad (2)$$

where $\frac{D\mathbf{R}}{D\mathbf{u}}$ is the tangent operator² and $\delta\mathbf{u}$ is the incremental response which is determined from the linear equation

$$\frac{D\mathbf{R}}{D\mathbf{u}}(\mathbf{u}^I)\delta\mathbf{u} = -\mathbf{R}(\mathbf{u}^I) \quad (3)$$

Upon evaluation of the incremental response $\delta\mathbf{u}$, the next iterate \mathbf{u}^{I+1} is updated from the sum

$$\mathbf{u}^{I+1} = \mathbf{u}^I + \delta\mathbf{u} \quad (4)$$

The process of evaluating the residual \mathbf{R} and updating the response \mathbf{u} continues until the solution converges, which for the Newton-Raphson method, is asymptotically quadratic.

In a sensitivity analysis, the residual \mathbf{R} and the system response \mathbf{u} are expressed as functions of the design parameter vector ϕ , i.e.

$$\mathbf{R}(\mathbf{u}(\phi), \phi) = \mathbf{0} \quad (5)$$

¹The system analysis, i.e. evaluation of a systems response, is referred to as the primal analysis throughout this document.

²Here and henceforth, we assume that all tangent operators are nonsingular.

The design parameters may be used to describe any of the analysis model input, e.g. material properties, load data and shape. A general response functional is then defined as

$$F(\phi) = G(\mathbf{u}(\phi), \phi) \quad (6)$$

This functional may be used to define cost or constraint functions in an optimization, or error functions in inverse and identification studies.

The sensitivity expression is obtained by differentiating equation (6) with respect to each component ϕ_i of ϕ , i.e.

$$\frac{DF}{D\phi_i} = \frac{\partial G}{\partial \mathbf{u}} \cdot \frac{D\mathbf{u}}{D\phi_i} + \frac{\partial G}{\partial \phi_i} \quad (7)$$

In the above equation, the derivatives $\frac{\partial G}{\partial \mathbf{u}}$ and $\frac{\partial G}{\partial \phi_i}$ are explicit quantities, whereas the derivative $\frac{D\mathbf{u}}{D\phi_i}$ is an implicit quantity because the system response is implicitly defined through equation (5).

2.1.1 Direct Differentiation Sensitivities for Steady-State Nonlinear Systems

In the direct differentiation approach, the implicit derivative $\frac{D\mathbf{u}}{D\phi_i}$ is evaluated and then the sensitivities are obtained from equation (7). This is accomplished by differentiating equation (5) with respect to the individual design parameters ϕ_i , which, after some rearranging, yields

$$\frac{\partial \mathbf{R}}{\partial \mathbf{u}} \frac{D\mathbf{u}}{D\phi_i} = -\frac{\partial \mathbf{R}}{\partial \phi_i} \quad (8)$$

The above equation forms a pseudo problem for the evaluation of the response sensitivity $\frac{D\mathbf{u}}{D\phi_i}$, resulting from the pseudo load $-\frac{\partial \mathbf{R}}{\partial \phi_i}$. Note here that the operator in the pseudo problem is identical to the tangent operator in the Newton-Raphson analysis of the primal problem (cf. equation (3)). In a finite element analysis, this reappearance of the tangent operator allows the decomposed tangent stiffness matrix resulting from the iterative solution of \mathbf{u} to be used to solve equation (8) efficiently for the implicit response sensitivity $\frac{D\mathbf{u}}{D\phi_i}$. Hence, the evaluation of the derivative $\frac{D\mathbf{u}}{D\phi_i}$ requires only the formation of the pseudo load vector $-\frac{\partial \mathbf{R}}{\partial \phi_i}$ for each design parameter ϕ_i , followed by a back substitution using the existing decomposed tangent stiffness matrix. Upon evaluating all response sensitivities $\frac{D\mathbf{u}}{D\phi_i}$, the sensitivities for any number of response functionals are evaluated from equation (7). As opposed to the finite difference sensitivity analysis, numerical implementation of the direct differentiation method adds only a small fraction to the overall computational cost.

2.1.2 Adjoint Sensitivities for Steady-State Nonlinear Systems

Adjoint sensitivities are obtained via the Lagrange multiplier method, where the implicit response sensitivity $\frac{D\mathbf{u}}{D\phi_i}$ is eliminated from equation (7). Equations (5) and (6) are combined to define the augmented functional

$$\hat{F}(\phi) \equiv G(\mathbf{u}(\phi), \phi) - \boldsymbol{\lambda}(\phi) \cdot \mathbf{R}(\mathbf{u}(\phi), \phi) \quad (9)$$

where $\boldsymbol{\lambda}(\phi)$ is the Lagrange multiplier and \mathbf{u} is a solution to equation (1). Note here that $\hat{F} = F$ since $\mathbf{R} = \mathbf{0}$ (cf. equation (5)). Differentiation of the above with respect to the individual design parameters ϕ_i yields

$$\begin{aligned} \frac{D\hat{F}}{D\phi_i} &= \frac{\partial G}{\partial \mathbf{u}} \cdot \frac{D\mathbf{u}}{D\phi_i} + \frac{\partial G}{\partial \phi_i} - \frac{D\boldsymbol{\lambda}}{D\phi_i} \cdot \mathbf{R} - \\ &\quad \boldsymbol{\lambda} \cdot \left(\frac{\partial \mathbf{R}}{\partial \mathbf{u}} \frac{D\mathbf{u}}{D\phi_i} + \frac{\partial \mathbf{R}}{\partial \phi_i} \right) \end{aligned} \quad (10)$$

Here, we note again that $\frac{D\hat{F}}{D\phi_i} = \frac{DF}{D\phi_i}$ since again $\mathbf{R} = \mathbf{0}$ and $\left(\frac{\partial \mathbf{R}}{\partial \mathbf{u}} \frac{D\mathbf{u}}{D\phi_i} + \frac{\partial \mathbf{R}}{\partial \phi_i} \right) = \mathbf{0}$ (cf. equations (5) and (8)).

To isolate the implicit response sensitivities, we separate equation (10) into two terms

$$\frac{D\hat{F}}{D\phi_i} = \frac{D\hat{F}_E}{D\phi_i} + \frac{D\hat{F}_I}{D\phi_i} \quad (11)$$

where $\frac{D\hat{F}_E}{D\phi_i}$ and $\frac{D\hat{F}_I}{D\phi_i}$ are the explicit and implicit terms, respectively, defined as

$$\frac{D\hat{F}_E}{D\phi_i} \equiv \frac{\partial G}{\partial \phi_i} - \boldsymbol{\lambda} \cdot \frac{\partial \mathbf{R}}{\partial \phi_i} \quad (12)$$

$$\frac{D\hat{F}_I}{D\phi_i} \equiv \frac{D\mathbf{u}}{D\phi_i} \cdot \left[\frac{\partial G}{\partial \mathbf{u}} - \left(\frac{\partial \mathbf{R}}{\partial \mathbf{u}} \right)^T \boldsymbol{\lambda} \right] \quad (13)$$

Here, $(\cdot)^T$ denotes the transpose operator. The implicit part $\frac{D\hat{F}_I}{D\phi_i}$ is eliminated from the sensitivity expression by defining the Lagrange multiplier $\boldsymbol{\lambda}$, so that equation (13) equals zero. Once this $\boldsymbol{\lambda}$ is determined, the unknown derivative $\frac{D\mathbf{u}}{D\phi_i}$ is eliminated from the sensitivity expression and the sensitivities are evaluated from the remaining explicit quantity (i.e. equation (12)). Annihilation of the implicit term (cf. equation (13)) yields the following adjoint problem for the adjoint response (Lagrange multiplier) $\boldsymbol{\lambda}$,

$$\left(\frac{\partial \mathbf{R}}{\partial \mathbf{u}} \right)^T \boldsymbol{\lambda} = \frac{\partial G}{\partial \mathbf{u}} \quad (14)$$

where $\frac{\partial G}{\partial \mathbf{u}}$ is deemed the adjoint load. Once the adjoint response $\boldsymbol{\lambda}$ is evaluated, the sensitivity expression reduces to

$$\frac{D\hat{F}}{D\phi_i} = \frac{\partial G}{\partial \phi_i} - \boldsymbol{\lambda} \cdot \frac{\partial \mathbf{R}}{\partial \phi_i} \quad (15)$$

Here, we note that the operator that appears in the adjoint problem is the transpose of the Newton-Raphson tangent operator used to obtain $\delta\mathbf{u}$ (cf. equation (3)). Therefore, in a finite element analysis, if the tangent stiffness matrix is symmetric, the decomposed tangent stiffness matrix resulting from the iterative solution of \mathbf{u} may be used to solve equation (14) efficiently. If the tangent stiffness is not symmetric, the adjoint problem may still be efficiently solved by standard LU decomposition techniques (cf. [38]).

The adjoint method requires the solution of one adjoint problem for each response functional F , whereby the sensitivity is computed from equation (15). Therefore, it is very efficient when the number of response functionals is small compared with the number of design parameters. If this ratio is reversed, the direct differentiation is generally preferred.

2.2 Transient Nonlinear Systems

For transient nonlinear problems, the response \mathbf{u} is a function of the time t . Additionally, the residual \mathbf{R} is a function of the time t , the response \mathbf{u} , and its time derivative³ $\dot{\mathbf{u}}$.

Numerical solutions of transient problems often necessitate that the time domain be discretized into a finite number of steps. For a typical time step, the time derivative of the response \mathbf{u} is approximated by the first-order finite difference⁴

$${}^n\dot{\mathbf{u}} \approx \frac{{}^n\mathbf{u} - {}^{n-1}\mathbf{u}}{{}^nt - {}^{n-1}t} \quad (16)$$

where the quantities ${}^{n-1}\mathbf{u}$ and ${}^n\mathbf{u}$ refer⁵ to the system response at the beginning and end of the time step n .

In light of the above, the residual ${}^n\mathbf{R}$, at time nt , is written as

$${}^n\mathbf{R}({}^n\mathbf{u}, {}^{n-1}\mathbf{u}) = \mathbf{0} \quad (17)$$

where ${}^{n-1}\mathbf{u}$ has been evaluated at the previous time step and ${}^n\mathbf{u}$ is yet to be determined. Here, the backward Euler integration scheme has been selected due to its inherent stability properties; however other schemes may also be incorporated (e.g. the variable midpoint algorithm [34]).

The Newton-Raphson process may again be used to evaluate the system response ${}^n\mathbf{u}$, just as in the steady-state case. Here, linearization of equation (17) yields the following linear equation for the incremental response $\delta\mathbf{u}$:

$$\frac{\partial {}^n\mathbf{R}}{\partial {}^n\mathbf{u}}({}^n\mathbf{u}^I)\delta\mathbf{u} = -{}^n\mathbf{R}({}^n\mathbf{u}^I) \quad (18)$$

³Higher order derivatives may be readily accommodated in this analysis.

⁴Higher order approximations may be accommodated in the analysis.

⁵Left superscripts denote the time at which the quantity is evaluated, i.e. ${}^nf = f({}^nt)$.

where we have suppressed ${}^{n-1}\mathbf{u}$ from the argument of \mathbf{R} as it is a fixed. The new estimate of the system response ${}^n\mathbf{u}^{I+1}$ is updated as

$${}^n\mathbf{u}^{I+1} = {}^n\mathbf{u}^I + \delta\mathbf{u} \quad (19)$$

and the process is repeated until the solution converges.

The sensitivity analysis parallels that of the steady-state case, where the residual ${}^n\mathbf{R}$, at time nt , is expressed as a function of the system response at the beginning and end of the time step and of the design ϕ , i.e.

$${}^n\mathbf{R}({}^n\mathbf{u}(\phi), {}^{n-1}\mathbf{u}(\phi), \phi) = \mathbf{0} \quad (20)$$

The response functional is defined here as a function of the terminal time Mt and the design ϕ ,

$$F(\phi) = G({}^M\mathbf{u}(\phi), \phi) \quad (21)$$

Note that the response functional could easily be defined as a function of all time nt , $n = 1, \dots, M$. (cf. [3]). However, for conciseness only the terminal response is considered.

The sensitivity is obtained by differentiating equation (21) with respect to each component ϕ_i of the design parameter vector ϕ , following the procedure of section 2.1, i.e.

$$\frac{DF}{D\phi_i} = \frac{\partial G}{\partial {}^M\mathbf{u}} \cdot \frac{D {}^M\mathbf{u}}{D\phi_i} + \frac{\partial G}{\partial \phi_i} \quad (22)$$

where the response sensitivity $\frac{D {}^M\mathbf{u}}{D\phi_i}$, is an implicit quantity defined through the residual at time Mt , (cf. equation (20) for $n = M$). To resolve this unknown quantity, either the direct differentiation or adjoint methods may be pursued.

2.2.1 Direct Differentiation Sensitivities for Transient Nonlinear Systems

Recall that in the direct differentiation method, the implicit response sensitivity $\frac{D {}^M\mathbf{u}}{D\phi_i}$, is evaluated by differentiating the residual (equation (20) at the terminal time Mt), which after some manipulation becomes

$$\frac{\partial {}^M\mathbf{R}}{\partial {}^M\mathbf{u}} \frac{D {}^M\mathbf{u}}{D\phi_i} = - \left(\frac{\partial {}^M\mathbf{R}}{\partial {}^{M-1}\mathbf{u}} \frac{D {}^{M-1}\mathbf{u}}{D\phi_i} + \frac{\partial {}^M\mathbf{R}}{\partial \phi_i} \right) \quad (23)$$

Equation (23) forms a pseudo problem for the evaluation of the response sensitivity $\frac{D {}^M\mathbf{u}}{D\phi_i}$, assuming that the derivative $\frac{D {}^{M-1}\mathbf{u}}{D\phi_i}$ is known. Here, we note that the operator in the pseudo problem is the tangent operator corresponding to the Newton-Raphson iteration for time step M . Thus, as in the steady-state case, the evaluation of $\frac{D {}^M\mathbf{u}}{D\phi_i}$ with the finite element

method, merely requires the formation of the pseudo load vector $-\left(\frac{\partial^M \mathbf{R}}{\partial^{M-1} \mathbf{u}} \frac{D^{M-1} \mathbf{u}}{D\phi_i} + \frac{\partial^M \mathbf{R}}{\partial \phi_i}\right)$, followed by a back substitution using the existing decomposed tangent stiffness matrix.

The derivative $\frac{D^{M-1} \mathbf{u}}{D\phi_i}$ in equation (23) is assumed to be a known quantity. This poses no difficulty as the derivative $\frac{D^{M-1} \mathbf{u}}{D\phi_i}$ may be evaluated by differentiating the residual equation at time ^{M-1}t , assuming that $\frac{D^{M-2} \mathbf{u}}{D\phi_i}$ is known. By decrementing this process, the derivative $\frac{D^1 \mathbf{u}}{D\phi_i}$ is at last evaluated by noting that the design derivative of the initial condition $\frac{D^0 \mathbf{u}}{D\phi_i}$ is known. These results are consistent with those in [39] which are derived in the continuous time domain and then discretized for computations. In [39], the pseudo problem is seen to be transient, which is also the present case.

In finite element applications, the response sensitivities $\frac{D^n \mathbf{u}}{D\phi_i}$, for $n = 1, \dots, M$, are evaluated simultaneously with the primal analysis, to reduce the computational cost. Upon convergence of the Newton-Raphson iterations, for each time step, the pseudo load vectors are formed and back substituted using the existing decomposed tangent stiffness matrix to evaluate the response sensitivity $\frac{D^n \mathbf{u}}{D\phi_i}$. The process is repeated at each time step until the terminal response sensitivity $\frac{D^M \mathbf{u}}{D\phi_i}$ is evaluated. Then, the sensitivity is computed from equation (22).

2.2.2 Adjoint Sensitivities for Transient Nonlinear Systems

Recall that the objective of the adjoint method is to eliminate the implicit response sensitivity $\frac{D^M \mathbf{u}}{D\phi_i}$ from the sensitivity expression (cf. equation (22)). By following the Lagrange multiplier method, equation (20) for all time $^n t$, $n = 1, \dots, M$, and equation (21) are combined to form the augmented functional

$$\begin{aligned} \hat{F}(\phi) &= G(^M \mathbf{u}(\phi), \phi) - ^M \boldsymbol{\lambda}(\phi) \cdot ^M \mathbf{R}(^M \mathbf{u}(\phi), ^{M-1} \mathbf{u}(\phi), \phi) \\ &\quad - ^{M-1} \boldsymbol{\lambda}(\phi) \cdot ^{M-1} \mathbf{R}(^{M-1} \mathbf{u}(\phi), ^{M-2} \mathbf{u}(\phi), \phi) \\ &\quad \dots \\ &\quad - ^1 \boldsymbol{\lambda}(\phi) \cdot ^1 \mathbf{R}(^1 \mathbf{u}(\phi), ^0 \mathbf{u}(\phi), \phi) \\ &= G(^M \mathbf{u}(\phi), \phi) - \sum_{n=1}^M ^n \boldsymbol{\lambda}(\phi) \cdot ^n \mathbf{R}(^n \mathbf{u}(\phi), ^{n-1} \mathbf{u}(\phi), \phi) \end{aligned} \quad (24)$$

where, $^1 \boldsymbol{\lambda}(\phi), ^2 \boldsymbol{\lambda}(\phi), \dots, ^M \boldsymbol{\lambda}(\phi)$ are the Lagrange multipliers which are actually the discretized solution of a transient adjoint problem at times $^n t$, $n = 1, \dots, M$. Again $\hat{F} = F$ since the residuals equal zero, i.e. $^n \mathbf{R} = \mathbf{0}$ for $n = 1, 2, \dots, M$, and $\frac{D\hat{F}}{D\phi_i} = \frac{DF}{D\phi_i}$ since again

${}^n\mathbf{R} = \mathbf{0}$ and $\frac{D^n\mathbf{R}}{D\phi_i} = \mathbf{0}$ (cf. equations (20) and (23)). Differentiation of equation (24) yields

$$\frac{D\hat{F}}{D\phi_i} = \frac{D\hat{F}_E}{D\phi_i} + \sum_{n=1}^M \frac{D^n\hat{F}_I}{D\phi_i} \quad (25)$$

where equation (20) is used above to eliminate the $\frac{D\lambda}{D\phi_i}$ terms and $\frac{D\hat{F}_E}{D\phi_i}$ contains the explicit terms while $\frac{D^1\hat{F}_I}{D\phi_i}, \frac{D^2\hat{F}_I}{D\phi_i}, \dots, \frac{D^M\hat{F}_I}{D\phi_i}$ contain the implicit quantities, i.e.

$$\frac{D\hat{F}_E}{D\phi_i} \equiv \frac{\partial G}{\partial \phi_i} - \sum_{n=1}^M {}^n\lambda \cdot \frac{\partial^n \mathbf{R}}{\partial \phi_i} - {}^1\lambda \cdot \frac{\partial^1 \mathbf{R}}{\partial^0 \mathbf{u}} \frac{D^0 \mathbf{u}}{D\phi_i} \quad (26)$$

and

$$\left. \begin{aligned} \frac{D^1\hat{F}_I}{D\phi_i} &\equiv -{}^1\lambda \cdot \frac{\partial^1 \mathbf{R}}{\partial^1 \mathbf{u}} \frac{D^1 \mathbf{u}}{D\phi_i} - {}^2\lambda \cdot \frac{\partial^2 \mathbf{R}}{\partial^1 \mathbf{u}} \frac{D^1 \mathbf{u}}{D\phi_i} \\ \frac{D^2\hat{F}_I}{D\phi_i} &\equiv -{}^2\lambda \cdot \frac{\partial^2 \mathbf{R}}{\partial^2 \mathbf{u}} \frac{D^2 \mathbf{u}}{D\phi_i} - {}^3\lambda \cdot \frac{\partial^3 \mathbf{R}}{\partial^2 \mathbf{u}} \frac{D^2 \mathbf{u}}{D\phi_i} \\ &\dots \\ \frac{D^{M-1}\hat{F}_I}{D\phi_i} &\equiv -{}^{M-1}\lambda \cdot \frac{\partial^{M-1} \mathbf{R}}{\partial^{M-1} \mathbf{u}} \frac{D^{M-1} \mathbf{u}}{D\phi_i} - {}^M\lambda \cdot \frac{\partial^M \mathbf{R}}{\partial^{M-1} \mathbf{u}} \frac{D^{M-1} \mathbf{u}}{D\phi_i} \\ \frac{D^M\hat{F}_I}{D\phi_i} &\equiv -{}^M\lambda \cdot \frac{\partial^M \mathbf{R}}{\partial^M \mathbf{u}} \frac{D^M \mathbf{u}}{D\phi_i} + \frac{\partial G}{\partial^M \mathbf{u}} \cdot \frac{D^M \mathbf{u}}{D\phi_i} \end{aligned} \right\} \quad (27)$$

The implicit system derivatives $\frac{D^1 \mathbf{u}}{D\phi_i}, \frac{D^2 \mathbf{u}}{D\phi_i}, \dots, \frac{D^M \mathbf{u}}{D\phi_i}$, are eliminated from the sensitivity expression by selecting the appropriate ${}^1\lambda(\phi), {}^2\lambda(\phi), \dots, {}^M\lambda(\phi)$ to annihilate the implicit quantities $\frac{D^1\hat{F}_I}{D\phi_i}, \frac{D^2\hat{F}_I}{D\phi_i}, \dots, \frac{D^M\hat{F}_I}{D\phi_i}$. From this process, we obtain the following set of adjoint problems:

$$\left. \begin{aligned} M &: \quad \left(\frac{\partial^M \mathbf{R}}{\partial^M \mathbf{u}} \right)^T {}^M\lambda = \frac{\partial G}{\partial^M \mathbf{u}} \\ M-1 &: \quad \left(\frac{\partial^{M-1} \mathbf{R}}{\partial^{M-1} \mathbf{u}} \right)^T {}^{M-1}\lambda = - \left(\frac{\partial^M \mathbf{R}}{\partial^{M-1} \mathbf{u}} \right)^T {}^M\lambda \\ &\dots \\ 2 &: \quad \left(\frac{\partial^2 \mathbf{R}}{\partial^2 \mathbf{u}} \right)^T {}^2\lambda = - \left(\frac{\partial^3 \mathbf{R}}{\partial^2 \mathbf{u}} \right)^T {}^3\lambda \\ 1 &: \quad \left(\frac{\partial^1 \mathbf{R}}{\partial^1 \mathbf{u}} \right)^T {}^1\lambda = - \left(\frac{\partial^2 \mathbf{R}}{\partial^1 \mathbf{u}} \right)^T {}^2\lambda \end{aligned} \right\} \quad (28)$$

Upon solving equations (28) for the adjoint responses ${}^1\lambda, {}^2\lambda, \dots, {}^M\lambda$, the sensitivity expression reduces to

$$\frac{D\hat{F}}{D\phi_i} = \frac{\partial G}{\partial \phi_i} - \sum_{n=1}^M {}^n\lambda \cdot \frac{\partial^n \mathbf{R}}{\partial \phi_i} - {}^1\lambda \cdot \frac{\partial^1 \mathbf{R}}{\partial^0 \mathbf{u}} \frac{D^0 \mathbf{u}}{D\phi_i} \quad (29)$$

Note here that the operators that appear in the adjoint problems of equations (28) are the transposes of the tangent operators of the Newton-Raphson solution procedure.

The evaluation of the adjoint sensitivities proceeds as follows: After the transient primal analysis is concluded, the adjoint response ${}^M \boldsymbol{\lambda}$ for the last time step is computed from the first of equations (28). Next, the adjoint response ${}^{M-1} \boldsymbol{\lambda}$ of the previous time step is computed from the second of equations (28). This process continues regressively until all adjoint responses are computed. Then, the sensitivities are computed from equation (29). The regressive computation of the adjoint response is consistent with the terminal adjoint problems in [3]. This is a consequence of the convolution operator used in transient variational statements [4, 40]. The use of nonuniform time steps in the continuous time domain approach of [41] causes complications; however, in the discrete approach shown here, no such complications arise.

For numerical applications, the adjoint method requires storage or recomputation of the converged decomposed tangent operators and the derivatives $\frac{\partial^2 \mathbf{R}}{\partial^2 \mathbf{u}}, \frac{\partial^3 \mathbf{R}}{\partial^3 \mathbf{u}}, \dots, \frac{\partial^M \mathbf{R}}{\partial^M \mathbf{u}}$, for every time step because the solution \mathbf{u} must be determined for all time before the adjoint analysis may begin. This increases either the computation or storage cost. However, when the design parameters significantly outnumber the response functionals, the adjoint method may still be preferred.

2.3 Steady-State Coupled Nonlinear Systems

Here, we consider steady-state nonlinear coupled systems which are expressed in residual form as

$$\mathbf{R}(\mathbf{u}, \mathbf{v}) = \mathbf{0} \quad (30)$$

$$\mathbf{H}(\mathbf{u}, \mathbf{v}) = \mathbf{0} \quad (31)$$

where \mathbf{R} and \mathbf{H} are residuals that must be simultaneously satisfied, and \mathbf{u} and \mathbf{v} are response fields.

The solution to the coupled problem may be achieved by assembling the residuals \mathbf{R} and \mathbf{H} into a single global residual \mathcal{R} , as

$$\mathcal{R}(\boldsymbol{u}) = \begin{bmatrix} \mathbf{R}(\mathbf{u}, \mathbf{v}) \\ \mathbf{H}(\mathbf{u}, \mathbf{v}) \end{bmatrix} = \mathbf{0} \quad (32)$$

where

$$\boldsymbol{u} = \begin{bmatrix} \mathbf{u} \\ \mathbf{v} \end{bmatrix} \quad (33)$$

and then following the analysis of section 2.1.

Another way to solve the coupled problem is to uncouple it by treating the response \mathbf{v} as a function of the system response \mathbf{u} . Then, the residuals of equations (30) and (31) are rewritten as

$$\mathbf{R}(\mathbf{u}, \mathbf{v}(\mathbf{u})) = \mathbf{0} \quad (34)$$

$$\mathbf{H}(\mathbf{u}, \mathbf{v}(\mathbf{u})) = \mathbf{0} \quad (35)$$

The solution of equations (34) and (35) is obtained by implementing the Newton-Raphson process in two nested iterative loops. In the outer loop, equation (34) is linearized yielding the following expression for the response correction $\delta\mathbf{u}$:

$$\left[\frac{\partial \mathbf{R}}{\partial \mathbf{u}}(\mathbf{u}^I, \mathbf{v}(\mathbf{u}^I)) + \frac{\partial \mathbf{R}}{\partial \mathbf{v}}(\mathbf{u}^I, \mathbf{v}(\mathbf{u}^I)) \frac{D\mathbf{v}}{D\mathbf{u}}(\mathbf{u}^I) \right] \delta\mathbf{u} = -\mathbf{R}(\mathbf{u}^I, \mathbf{v}(\mathbf{u}^I)) \quad (36)$$

However, before equation (36) may be solved, both the system response $\mathbf{v}(\mathbf{u}^I)$ and the derivative $\frac{D\mathbf{v}}{D\mathbf{u}}(\mathbf{u}^I)$ must be determined.

The evaluation of $\mathbf{v}(\mathbf{u}^I)$ is performed in the inner loop by solving equation (35) for $\mathbf{v}(\mathbf{u}^I)$ via the Newton-Raphson process where the current iterate \mathbf{u}^I is fixed. Linearization of equation (35) about the current iterate $\mathbf{v}^J(\mathbf{u}^I)$, for a fixed \mathbf{u}^I , yields the following equation for the incremental response $\delta\mathbf{v}$:

$$\frac{\partial \mathbf{H}}{\partial \mathbf{v}}(\mathbf{u}^I, \mathbf{v}^J(\mathbf{u}^I)) \delta\mathbf{v} = -\mathbf{H}(\mathbf{u}^I, \mathbf{v}^J(\mathbf{u}^I)) \quad (37)$$

where $\frac{\partial \mathbf{H}}{\partial \mathbf{v}}$ is deemed the dependent tangent operator. Upon evaluating the incremental response $\delta\mathbf{v}$, the next iterate $\mathbf{v}^{J+1}(\mathbf{u}^I)$ is computed from

$$\mathbf{v}^{J+1}(\mathbf{u}^I) = \mathbf{v}^J(\mathbf{u}^I) + \delta\mathbf{v} \quad (38)$$

The Newton-Raphson subiterations are repeated for this inner loop until they converge to the solution $\mathbf{v}(\mathbf{u}^I)$.

Once $\mathbf{v}(\mathbf{u}^I)$ is determined, the derivative $\frac{D\mathbf{v}}{D\mathbf{u}}(\mathbf{u}^I)$ is obtained by differentiating equation (35), i.e.

$$\frac{\partial \mathbf{H}}{\partial \mathbf{u}}(\mathbf{u}^I, \mathbf{v}(\mathbf{u}^I)) + \frac{\partial \mathbf{H}}{\partial \mathbf{v}}(\mathbf{u}^I, \mathbf{v}(\mathbf{u}^I)) \frac{D\mathbf{v}}{D\mathbf{u}}(\mathbf{u}^I) = \mathbf{0} \quad (39)$$

whereupon $\frac{D\mathbf{v}}{D\mathbf{u}}(\mathbf{u}^I)$ is computed from

$$\frac{D\mathbf{v}}{D\mathbf{u}}(\mathbf{u}^I) = - \left(\frac{\partial \mathbf{H}}{\partial \mathbf{v}}(\mathbf{u}^I, \mathbf{v}(\mathbf{u}^I)) \right)^{-1} \frac{\partial \mathbf{H}}{\partial \mathbf{u}}(\mathbf{u}^I, \mathbf{v}(\mathbf{u}^I)) \quad (40)$$

Note here that the dependent operator $\frac{\partial \mathbf{H}}{\partial \mathbf{v}}(\mathbf{u}^I, \mathbf{v}(\mathbf{u}^I))$ has been previously decomposed in the computation of the incremental response $\delta\mathbf{v}$ (cf. equation (37)). Thus, $\frac{D\mathbf{v}}{D\mathbf{u}}(\mathbf{u}^I)$ may be efficiently computed by a series of back substitutions.

Upon evaluation of $\mathbf{v}(\mathbf{u}^I)$ and $\frac{D\mathbf{v}}{D\mathbf{u}}(\mathbf{u}^I)$ the inner loop is completed. Equation (40) is then substituted into equation (36) to obtain

$$\left[\frac{\partial \mathbf{R}}{\partial \mathbf{u}}(\mathbf{u}^I, \mathbf{v}(\mathbf{u}^I)) - \frac{\partial \mathbf{R}}{\partial \mathbf{v}}(\mathbf{u}^I, \mathbf{v}(\mathbf{u}^I)) \overbrace{\left(\frac{\partial \mathbf{H}}{\partial \mathbf{v}}(\mathbf{u}^I, \mathbf{v}(\mathbf{u}^I)) \right)^{-1} \frac{\partial \mathbf{H}}{\partial \mathbf{u}}(\mathbf{u}^I, \mathbf{v}(\mathbf{u}^I))}^{-\frac{\partial^{n\mathbf{v}}}{\partial^{n\mathbf{u}}}(\mathbf{u}^I)} \right] \delta \mathbf{u} = -\mathbf{R}(\mathbf{u}^I, \mathbf{v}(\mathbf{u}^I)) \quad (41)$$

where the term in brackets is deemed the independent tangent operator. The system response is then updated from the sum

$$\mathbf{u}^{I+1} = \mathbf{u}^I + \delta \mathbf{u} \quad (42)$$

The iteration-subiteration process is repeated for each iterate \mathbf{u}^I , until equation (34) converges (cf. figure (1)).

For the sensitivity analysis, the response fields \mathbf{u} and \mathbf{v} are defined as functions of the design ϕ . The residuals of equations (30) and (31) are then rewritten as

$$\mathbf{R}(\mathbf{u}(\phi), \mathbf{v}(\phi), \phi) = \mathbf{0} \quad (43)$$

and

$$\mathbf{H}(\mathbf{u}(\phi), \mathbf{v}(\phi), \phi) = \mathbf{0} \quad (44)$$

and the response functional becomes

$$F(\phi) = G(\mathbf{u}(\phi), \mathbf{v}(\phi), \phi) \quad (45)$$

As in section 2.1, the sensitivity expression is obtained by differentiating equation (45) with respect to each design parameter ϕ_i , i.e.

$$\frac{DF}{D\phi_i} = \frac{\partial G}{\partial \mathbf{u}} \cdot \frac{D\mathbf{u}}{D\phi_i} + \frac{\partial G}{\partial \mathbf{v}} \cdot \frac{D\mathbf{v}}{D\phi_i} + \frac{\partial G}{\partial \phi_i} \quad (46)$$

where now the response sensitivities $\frac{D\mathbf{u}}{D\phi_i}$ and $\frac{D\mathbf{v}}{D\phi_i}$ are implicitly defined through equations (43) and (44).

2.3.1 Direct Differentiation Sensitivities for Steady-State Coupled Nonlinear Systems

As in the direct differentiation sensitivity analysis for uncoupled systems, the objective here is to compute the sensitivity analytically by evaluating the implicit response sensitivities $\frac{D\mathbf{u}}{D\phi_i}$

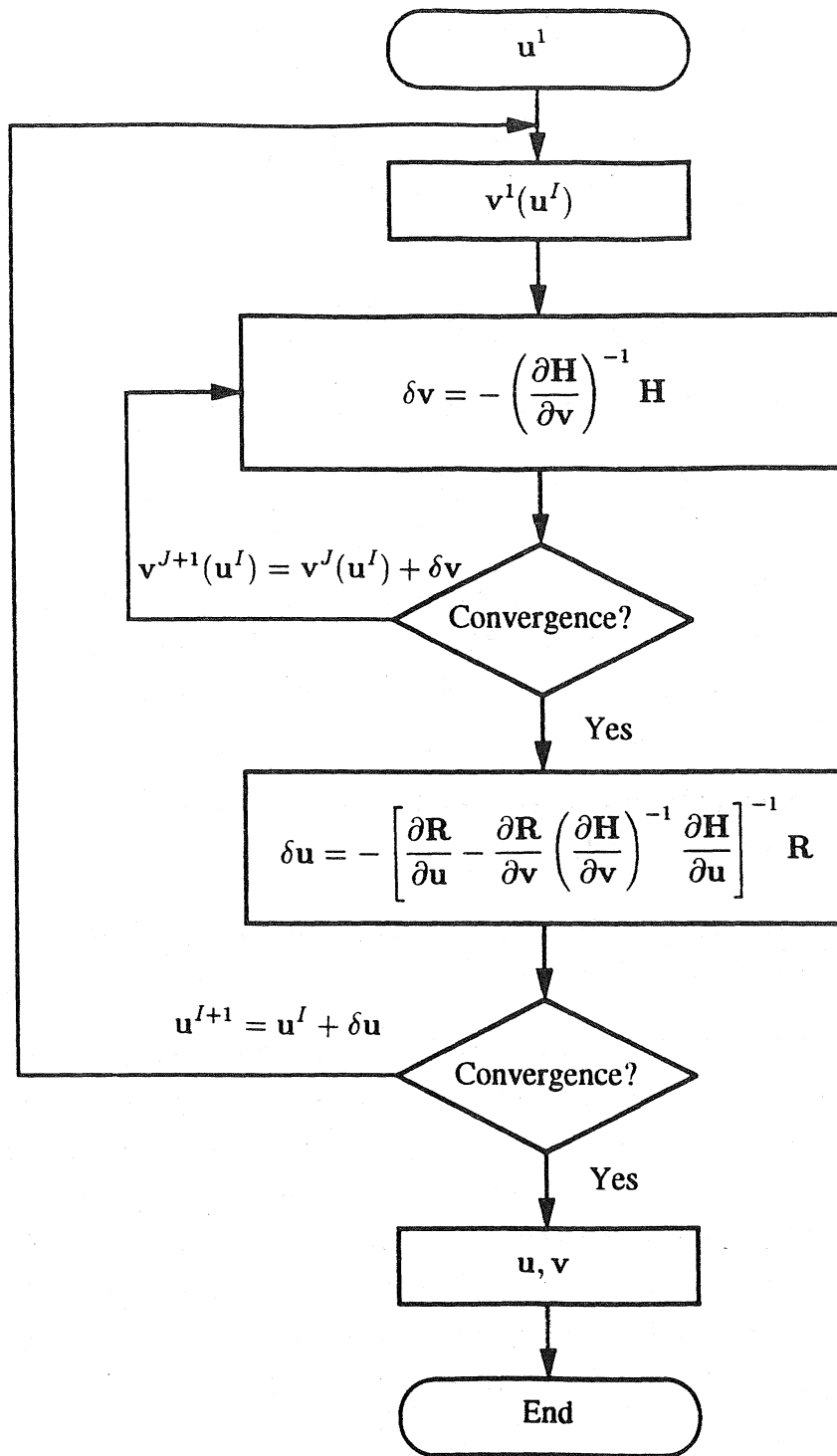


Figure 1: Newton-Raphson iteration-subiteration process.

and $\frac{D\mathbf{v}}{D\phi_i}$. To this end, we differentiate the residual equations (43) and (44) with respect to each design parameter ϕ_i , i.e.

$$\frac{\partial \mathbf{R}}{\partial \mathbf{u}} \frac{D\mathbf{u}}{D\phi_i} + \frac{\partial \mathbf{R}}{\partial \mathbf{v}} \frac{D\mathbf{v}}{D\phi_i} + \frac{\partial \mathbf{R}}{\partial \phi_i} = \mathbf{0} \quad (47)$$

and

$$\frac{\partial \mathbf{H}}{\partial \mathbf{u}} \frac{D\mathbf{u}}{D\phi_i} + \frac{\partial \mathbf{H}}{\partial \mathbf{v}} \frac{D\mathbf{v}}{D\phi_i} + \frac{\partial \mathbf{H}}{\partial \phi_i} = \mathbf{0} \quad (48)$$

The implicit derivative $\frac{D\mathbf{v}}{D\phi_i}$ is determined by rearranging equation (48) as

$$\frac{D\mathbf{v}}{D\phi_i} = - \left(\frac{\partial \mathbf{H}}{\partial \mathbf{v}} \right)^{-1} \left[\frac{\partial \mathbf{H}}{\partial \mathbf{u}} \frac{D\mathbf{u}}{D\phi_i} + \frac{\partial \mathbf{H}}{\partial \phi_i} \right] \quad (49)$$

where the operator $\frac{\partial \mathbf{H}}{\partial \mathbf{v}}$ is the dependent tangent operator used in the Newton-Raphson subiteration process for the evaluation of the incremental response $\delta \mathbf{v}$ (cf. equation (37)). Here, $\frac{D\mathbf{v}}{D\phi_i}$ is deemed the dependent response sensitivity as it is dependent on the derivative $\frac{D\mathbf{u}}{D\phi_i}$ as seen through equation (49).

Substituting equation (49) into equation (47) we obtain the following expression for the independent response sensitivity $\frac{D\mathbf{u}}{D\phi_i}$:

$$\left[\frac{\partial \mathbf{R}}{\partial \mathbf{u}} - \frac{\partial \mathbf{R}}{\partial \mathbf{v}} \left(\frac{\partial \mathbf{H}}{\partial \mathbf{v}} \right)^{-1} \frac{\partial \mathbf{H}}{\partial \mathbf{u}} \right] \frac{D\mathbf{u}}{D\phi_i} = - \left[\frac{\partial \mathbf{R}}{\partial \phi_i} - \frac{\partial \mathbf{R}}{\partial \mathbf{v}} \left(\frac{\partial \mathbf{H}}{\partial \mathbf{v}} \right)^{-1} \frac{\partial \mathbf{H}}{\partial \phi_i} \right] \quad (50)$$

where the left-hand side bracketed operator is the independent tangent operator of equation (41). Upon evaluation of the independent derivative $\frac{D\mathbf{u}}{D\phi_i}$, the dependent derivative $\frac{D\mathbf{v}}{D\phi_i}$ is computed from equation (49), and then the sensitivity is evaluated from equation (46). In finite element applications, for each design parameter the direct method requires two pseudo load formations and two back substitutions using the existing decomposed tangent operators. This sensitivity formulation is consistent with the coupled thermoelastic and contact sensitivity formulations of [22, 42]. Finally, note that the order in which the dependent and independent pseudo problems are solved is reversed that of the primal incremental problems.

2.3.2 Adjoint Sensitivities for Steady-State Coupled Nonlinear Systems

The augmented functional \hat{F} for the adjoint sensitivity method is obtained by combining equations (43) through (45) and introducing two Lagrange multipliers $\boldsymbol{\lambda}$ and $\boldsymbol{\gamma}$, i.e.

$$\hat{F}(\boldsymbol{\phi}) \equiv G(\mathbf{u}(\boldsymbol{\phi}), \mathbf{v}(\boldsymbol{\phi}), \boldsymbol{\phi}) - \boldsymbol{\lambda}(\boldsymbol{\phi}) \cdot \mathbf{R}(\mathbf{u}(\boldsymbol{\phi}), \mathbf{v}(\boldsymbol{\phi}), \boldsymbol{\phi}) - \boldsymbol{\gamma}(\boldsymbol{\phi}) \cdot \mathbf{H}(\mathbf{u}(\boldsymbol{\phi}), \mathbf{v}(\boldsymbol{\phi}), \boldsymbol{\phi}) \quad (51)$$

Differentiation of the above equation with respect to the design parameter ϕ_i , gives

$$\begin{aligned} \frac{D\hat{F}}{D\phi_i} &= \frac{\partial G}{\partial \mathbf{u}} \cdot \frac{D\mathbf{u}}{D\phi_i} + \frac{\partial G}{\partial \mathbf{v}} \cdot \frac{D\mathbf{v}}{D\phi_i} + \frac{\partial G}{\partial \phi_i} - \\ &\quad \frac{D\boldsymbol{\lambda}}{D\phi_i} \cdot \mathbf{R} - \boldsymbol{\lambda} \cdot \left(\frac{\partial \mathbf{R}}{\partial \mathbf{u}} \frac{D\mathbf{u}}{D\phi_i} + \frac{\partial \mathbf{R}}{\partial \mathbf{v}} \frac{D\mathbf{v}}{D\phi_i} + \frac{\partial \mathbf{R}}{\partial \phi_i} \right) - \\ &\quad \frac{D\boldsymbol{\gamma}}{D\phi_i} \cdot \mathbf{H} - \boldsymbol{\gamma} \cdot \left(\frac{\partial \mathbf{H}}{\partial \mathbf{u}} \frac{D\mathbf{u}}{D\phi_i} + \frac{\partial \mathbf{H}}{\partial \mathbf{v}} \frac{D\mathbf{v}}{D\phi_i} + \frac{\partial \mathbf{H}}{\partial \phi_i} \right) \end{aligned} \quad (52)$$

The explicit and implicit quantities in equation (52) are isolated, i.e.

$$\frac{D\hat{F}}{D\phi_i} = \frac{D\hat{F}_E}{D\phi_i} + \left(\frac{D\hat{F}_I}{D\phi_i} \right)_{\boldsymbol{\lambda}} + \left(\frac{D\hat{F}_I}{D\phi_i} \right)_{\boldsymbol{\gamma}} \quad (53)$$

where

$$\frac{D\hat{F}_E}{D\phi_i} \equiv \frac{\partial G}{\partial \phi_i} - \boldsymbol{\lambda} \cdot \frac{\partial \mathbf{R}}{\partial \phi_i} - \boldsymbol{\gamma} \cdot \frac{\partial \mathbf{H}}{\partial \phi_i} \quad (54)$$

and

$$\left(\frac{D\hat{F}_I}{D\phi_i} \right)_{\boldsymbol{\lambda}} \equiv \frac{D\mathbf{u}}{D\phi_i} \cdot \left[\frac{\partial G}{\partial \mathbf{u}} - \left(\frac{\partial \mathbf{R}}{\partial \mathbf{u}} \right)^T \boldsymbol{\lambda} - \left(\frac{\partial \mathbf{H}}{\partial \mathbf{u}} \right)^T \boldsymbol{\gamma} \right] \quad (55)$$

and

$$\left(\frac{D\hat{F}_I}{D\phi_i} \right)_{\boldsymbol{\gamma}} \equiv \frac{D\mathbf{v}}{D\phi_i} \cdot \left[\frac{\partial G}{\partial \mathbf{v}} - \left(\frac{\partial \mathbf{R}}{\partial \mathbf{v}} \right)^T \boldsymbol{\lambda} - \left(\frac{\partial \mathbf{H}}{\partial \mathbf{v}} \right)^T \boldsymbol{\gamma} \right]. \quad (56)$$

Here $\frac{D\hat{F}_E}{D\phi_i}$ is the explicit quantity and $\left(\frac{D\hat{F}_I}{D\phi_i} \right)_{\boldsymbol{\lambda}}$ and $\left(\frac{D\hat{F}_I}{D\phi_i} \right)_{\boldsymbol{\gamma}}$ are the implicit quantities.

The implicit sensitivity quantities $\left(\frac{D\hat{F}_I}{D\phi_i} \right)_{\boldsymbol{\lambda}}$ and $\left(\frac{D\hat{F}_I}{D\phi_i} \right)_{\boldsymbol{\gamma}}$, are equated to zero to eliminate the unknown response sensitivities $\frac{D\mathbf{u}}{D\phi_i}$ and $\frac{D\mathbf{v}}{D\phi_i}$, from the sensitivity expression, by following the adjoint approach of the previous sections. This yields the following coupled adjoint problem for the Lagrange multipliers $\boldsymbol{\lambda}$ and $\boldsymbol{\gamma}$:

$$\left(\frac{\partial \mathbf{R}}{\partial \mathbf{u}} \right)^T \boldsymbol{\lambda} + \left(\frac{\partial \mathbf{H}}{\partial \mathbf{u}} \right)^T \boldsymbol{\gamma} = \frac{\partial G}{\partial \mathbf{u}} \quad (57)$$

$$\left(\frac{\partial \mathbf{R}}{\partial \mathbf{v}} \right)^T \boldsymbol{\lambda} + \left(\frac{\partial \mathbf{H}}{\partial \mathbf{v}} \right)^T \boldsymbol{\gamma} = \frac{\partial G}{\partial \mathbf{v}} \quad (58)$$

The adjoint problem is uncoupled by treating the dependent adjoint response $\boldsymbol{\gamma}$ as function of the independent adjoint response $\boldsymbol{\lambda}$, i.e. $\boldsymbol{\gamma} = \boldsymbol{\gamma}(\boldsymbol{\lambda})$. Rearrangement of equation (58) then yields the dependent adjoint problem

$$\boldsymbol{\gamma} = \left(\frac{\partial \mathbf{H}}{\partial \mathbf{v}} \right)^{-T} \left[\frac{\partial G}{\partial \mathbf{v}} - \left(\frac{\partial \mathbf{R}}{\partial \mathbf{v}} \right)^T \boldsymbol{\lambda} \right] \quad (59)$$

where the left-hand side operator above is the inverse transpose of the dependent Newton-Raphson tangent operator (cf. equation (37)). Substitution of equation (59) into equation (57) yields the following independent adjoint problem for λ :

$$\left[\frac{\partial \mathbf{R}}{\partial \mathbf{u}} - \frac{\partial \mathbf{R}}{\partial \mathbf{v}} \left(\frac{\partial \mathbf{H}}{\partial \mathbf{v}} \right)^{-1} \frac{\partial \mathbf{H}}{\partial \mathbf{u}} \right]^T \lambda = \left[\frac{\partial G}{\partial \mathbf{u}} - \left[\left(\frac{\partial \mathbf{H}}{\partial \mathbf{v}} \right)^{-1} \frac{\partial \mathbf{H}}{\partial \mathbf{u}} \right]^T \frac{\partial G}{\partial \mathbf{v}} \right] \quad (60)$$

In the above equation, the left-hand side operator is the transpose of the independent Newton-Raphson tangent operator (cf. equation (41)), and the right-hand side term forms the independent adjoint load. Upon evaluation of the independent adjoint response λ , from equation (60), the dependent adjoint response γ is computed by forming the dependent adjoint load $\left(\frac{\partial G}{\partial \mathbf{v}} - \left(\frac{\partial \mathbf{R}}{\partial \mathbf{v}} \right)^T \lambda \right)$ and evaluating equation (59). Once λ and γ are evaluated, the sensitivity expression for the adjoint method is reduced to equation (54). This adjoint sensitivity formulation is consistent with the thermoelastic sensitivity formulation of [23]. Again, note the solution order of the dependent and independent adjoint problems is reversed that of the primal incremental problems.

For finite element applications, the tangent stiffness matrices for the adjoint problems are the transposes of the Newton-Raphson tangent stiffness matrices of the primal analysis. Therefore, for every response functional, the adjoint method requires two formations of the adjoint load vectors and two back substitutions using the existing decomposed tangent stiffness matrices.

2.4 Transient Coupled Nonlinear Systems

For transient coupled systems, the residuals ${}^n\mathbf{R}$ and ${}^n\mathbf{H}$ at time nt are expressed as

$${}^n\mathbf{R}({}^n\mathbf{u}, {}^{n-1}\mathbf{u}, {}^n\mathbf{v}, {}^{n-1}\mathbf{v}) = \mathbf{0} \quad (61)$$

and

$${}^n\mathbf{H}({}^n\mathbf{u}, {}^{n-1}\mathbf{u}, {}^n\mathbf{v}, {}^{n-1}\mathbf{v}) = \mathbf{0} \quad (62)$$

As in section 2.3, the responses ${}^{n-1}\mathbf{u}$ and ${}^{n-1}\mathbf{v}$ are known quantities and equations (61) and (62) are solved for ${}^n\mathbf{u}$ and ${}^n\mathbf{v}$. Now, by suppressing the $n - 1$ terms for conciseness and by following the analyses of the previous sections, the system is uncoupled by treating the response ${}^n\mathbf{v}$ as function of the response ${}^n\mathbf{u}$. Then, equations (61) and (62) are rewritten as

$${}^n\mathbf{R}({}^n\mathbf{u}, {}^n\mathbf{v}({}^n\mathbf{u})) = \mathbf{0} \quad (63)$$

and

$${}^n\mathbf{H}({}^n\mathbf{u}, {}^n\mathbf{v}({}^n\mathbf{u})) = \mathbf{0} \quad (64)$$

This system is now solved for ${}^n\mathbf{u}$ and ${}^n\mathbf{v}$ by applying the iteration-subiteration method presented in section 2.3.

The sensitivity analysis of transient coupled nonlinear systems follows that of sections 2.2 and 2.3. The residuals of equations (61) and (62) are rewritten as

$${}^n\mathbf{R}({}^n\mathbf{u}(\phi), {}^{n-1}\mathbf{u}(\phi), {}^n\mathbf{v}(\phi), {}^{n-1}\mathbf{v}(\phi), \phi) = \mathbf{0} \quad (65)$$

and

$${}^n\mathbf{H}({}^n\mathbf{u}(\phi), {}^{n-1}\mathbf{u}(\phi), {}^n\mathbf{v}(\phi), {}^{n-1}\mathbf{v}(\phi), \phi) = \mathbf{0} \quad (66)$$

and the response functional F is defined as⁶

$$F(\phi) = G({}^M\mathbf{u}(\phi), {}^M\mathbf{v}(\phi), \phi) \quad (67)$$

The sensitivity expression is obtained from

$$\frac{DF}{D\phi_i} = \frac{\partial G}{\partial {}^M\mathbf{u}} \cdot \frac{D {}^M\mathbf{u}}{D\phi_i} + \frac{\partial G}{\partial {}^M\mathbf{v}} \cdot \frac{D {}^M\mathbf{v}}{D\phi_i} + \frac{\partial G}{\partial \phi_i} \quad (68)$$

where $\frac{D {}^M\mathbf{u}}{D\phi_i}$ and $\frac{D {}^M\mathbf{v}}{D\phi_i}$ are the implicit response sensitivities.

2.4.1 Direct Differentiation Sensitivities for Transient Coupled Nonlinear Systems

To evaluate the implicit derivatives $\frac{D {}^n\mathbf{u}}{D\phi_i}$ and $\frac{D {}^n\mathbf{v}}{D\phi_i}$, we express the derivative $\frac{D {}^M\mathbf{v}}{D\phi_i}$ in terms of the derivative $\frac{D {}^M\mathbf{u}}{D\phi_i}$, by differentiating equation (66) for $n = M$, i.e.

$$\frac{D {}^M\mathbf{v}}{D\phi_i} = - \left(\frac{\partial {}^M\mathbf{H}}{\partial {}^M\mathbf{v}} \right)^{-1} \left[\frac{\partial {}^M\mathbf{H}}{\partial {}^M\mathbf{u}} \frac{D {}^M\mathbf{u}}{D\phi_i} + \frac{\partial {}^M\mathbf{H}}{\partial {}^{M-1}\mathbf{u}} \frac{D {}^{M-1}\mathbf{u}}{D\phi_i} + \frac{\partial {}^M\mathbf{H}}{\partial {}^{M-1}\mathbf{v}} \frac{D {}^{M-1}\mathbf{v}}{D\phi_i} + \frac{\partial {}^M\mathbf{H}}{\partial \phi_i} \right] \quad (69)$$

where $\frac{\partial {}^M\mathbf{H}}{\partial {}^M\mathbf{v}}$ is the dependent tangent operator and the right-hand side bracketed term forms the dependent pseudo load.

Differentiation of equation (65) and use of equation (69) yields

$$\begin{aligned} & \left[\frac{\partial {}^M\mathbf{R}}{\partial {}^M\mathbf{u}} - \frac{\partial {}^M\mathbf{R}}{\partial {}^M\mathbf{v}} \left(\frac{\partial {}^M\mathbf{H}}{\partial {}^M\mathbf{v}} \right)^{-1} \frac{\partial {}^M\mathbf{H}}{\partial {}^M\mathbf{u}} \right] \frac{D {}^M\mathbf{u}}{D\phi_i} = \\ & - \left[\frac{\partial {}^M\mathbf{R}}{\partial {}^{M-1}\mathbf{u}} \frac{D {}^{M-1}\mathbf{u}}{D\phi_i} + \frac{\partial {}^M\mathbf{R}}{\partial {}^{M-1}\mathbf{v}} \frac{D {}^{M-1}\mathbf{v}}{D\phi_i} + \frac{\partial {}^M\mathbf{R}}{\partial \phi_i} \right. \\ & \left. - \frac{\partial {}^M\mathbf{R}}{\partial {}^M\mathbf{v}} \left(\frac{\partial {}^M\mathbf{H}}{\partial {}^M\mathbf{v}} \right)^{-1} \left(\frac{\partial {}^M\mathbf{H}}{\partial \phi_i} + \frac{\partial {}^M\mathbf{H}}{\partial {}^{M-1}\mathbf{u}} \frac{D {}^{M-1}\mathbf{u}}{D\phi_i} + \frac{\partial {}^M\mathbf{H}}{\partial {}^{M-1}\mathbf{v}} \frac{D {}^{M-1}\mathbf{v}}{D\phi_i} \right) \right] \quad (70) \end{aligned}$$

⁶Again, F may be defined on all time, but a terminal expression is assumed here for conciseness (cf. section 2.2).

In the above independent pseudo problem for the response sensitivity $\frac{D^M \mathbf{u}}{D\phi_i}$, the left-hand side bracketed operator is the independent tangent operator and the right-hand side forms the independent pseudo load. Once $\frac{D^M \mathbf{u}}{D\phi_i}$ is evaluated, $\frac{D^M \mathbf{v}}{D\phi_i}$ is determined from equation (69) after which the sensitivity is computed from equation (68). The formation of the pseudo loads requires the computation of the derivatives $\frac{D^{M-1} \mathbf{u}}{D\phi_i}$ and $\frac{D^{M-1} \mathbf{v}}{D\phi_i}$, which is obtained by following the transient direct differentiation process discussed in section 2.2.1.

Finite element application of the direct differentiation method follows from section 2.2.1. It requires two back substitutions using existing decomposed stiffness matrices of the primal analysis, for each time step and for each design parameter. This sensitivity formulation is consistent with the rate-independent elasto-plastic sensitivity formulation of [34].

2.4.2 Adjoint Sensitivities for Transient Coupled Nonlinear Systems

In the adjoint sensitivity formulation, equations (65), (66) and (67) are combined to form the augmented response functional

$$\begin{aligned} \hat{F}(\phi) \equiv & G({}^M \mathbf{u}(\phi), {}^M \mathbf{v}(\phi), \phi) - \sum_{n=1}^M {}^n \boldsymbol{\lambda} \cdot {}^n \mathbf{R}({}^n \mathbf{u}(\phi), {}^{n-1} \mathbf{u}(\phi), {}^n \mathbf{v}(\phi), {}^{n-1} \mathbf{v}(\phi), \phi) - \\ & \sum_{n=1}^M {}^n \boldsymbol{\gamma} \cdot {}^n \mathbf{H}({}^n \mathbf{u}(\phi), {}^{n-1} \mathbf{u}(\phi), {}^n \mathbf{v}(\phi), {}^{n-1} \mathbf{v}(\phi), \phi) \end{aligned} \quad (71)$$

where ${}^n \boldsymbol{\lambda}$ and ${}^n \boldsymbol{\gamma}$ are arbitrary Lagrange multipliers.

Differentiation of equation (71) with respect to the design parameters ϕ_i yields the following sensitivity expression:

$$\frac{D \hat{F}}{D \phi_i} = \frac{D \hat{F}_E}{D \phi_i} + \sum_{n=1}^M \left(\frac{D {}^n \hat{F}_I}{D \phi_i} \right)_{\boldsymbol{\lambda}} + \sum_{n=1}^M \left(\frac{D {}^n \hat{F}_I}{D \phi_i} \right)_{\boldsymbol{\gamma}} \quad (72)$$

where $\frac{D \hat{F}_E}{D \phi_i}$ is explicit and $\left(\frac{D {}^n \hat{F}_I}{D \phi_i} \right)_{\boldsymbol{\lambda}}$ and $\left(\frac{D {}^n \hat{F}_I}{D \phi_i} \right)_{\boldsymbol{\gamma}}$ are implicit terms, defined as

$$\begin{aligned} \frac{D \hat{F}_E}{D \phi_i} \equiv & \frac{\partial G}{\partial \phi_i} - \sum_{n=1}^M {}^n \boldsymbol{\lambda} \cdot \frac{\partial {}^n \mathbf{R}}{\partial \phi_i} - {}^1 \boldsymbol{\lambda} \cdot \frac{\partial {}^1 \mathbf{R}}{\partial {}^0 \mathbf{u}} \frac{D {}^0 \mathbf{u}}{D \phi_i} - {}^1 \boldsymbol{\lambda} \cdot \frac{\partial {}^1 \mathbf{R}}{\partial {}^0 \mathbf{v}} \frac{D {}^0 \mathbf{v}}{D \phi_i} - \\ & \sum_{n=1}^M {}^n \boldsymbol{\gamma} \cdot \frac{\partial {}^n \mathbf{H}}{\partial \phi_i} - {}^1 \boldsymbol{\gamma} \cdot \frac{\partial {}^1 \mathbf{H}}{\partial {}^0 \mathbf{u}} \frac{D {}^0 \mathbf{u}}{D \phi_i} - {}^1 \boldsymbol{\gamma} \cdot \frac{\partial {}^1 \mathbf{H}}{\partial {}^0 \mathbf{v}} \frac{D {}^0 \mathbf{v}}{D \phi_i} \end{aligned} \quad (73)$$

and

$$\begin{aligned}
 \left(\frac{D^1 \hat{F}_I}{D\phi_i} \right)_{\lambda} &\equiv - \left[{}^1\lambda \cdot \frac{\partial^1 \mathbf{R}}{\partial^1 \mathbf{u}} + {}^1\gamma \cdot \frac{\partial^1 \mathbf{H}}{\partial^1 \mathbf{u}} + {}^2\lambda \cdot \frac{\partial^2 \mathbf{R}}{\partial^1 \mathbf{u}} + {}^2\gamma \cdot \frac{\partial^2 \mathbf{H}}{\partial^1 \mathbf{u}} \right] \frac{D^1 \mathbf{u}}{D\phi_i} \\
 \left(\frac{D^1 \hat{F}_I}{D\phi_i} \right)_{\gamma} &\equiv - \left[{}^1\lambda \cdot \frac{\partial^1 \mathbf{R}}{\partial^1 \mathbf{v}} + {}^1\gamma \cdot \frac{\partial^1 \mathbf{H}}{\partial^1 \mathbf{v}} + {}^2\lambda \cdot \frac{\partial^2 \mathbf{R}}{\partial^1 \mathbf{v}} + {}^2\gamma \cdot \frac{\partial^2 \mathbf{H}}{\partial^1 \mathbf{v}} \right] \frac{D^1 \mathbf{v}}{D\phi_i} \\
 \left(\frac{D^2 \hat{F}_I}{D\phi_i} \right)_{\lambda} &\equiv - \left[{}^2\lambda \cdot \frac{\partial^2 \mathbf{R}}{\partial^2 \mathbf{u}} + {}^2\gamma \cdot \frac{\partial^2 \mathbf{H}}{\partial^2 \mathbf{u}} + {}^3\lambda \cdot \frac{\partial^3 \mathbf{R}}{\partial^2 \mathbf{u}} + {}^3\gamma \cdot \frac{\partial^3 \mathbf{H}}{\partial^2 \mathbf{u}} \right] \frac{D^2 \mathbf{u}}{D\phi_i} \\
 \left(\frac{D^2 \hat{F}_I}{D\phi_i} \right)_{\gamma} &\equiv - \left[{}^2\lambda \cdot \frac{\partial^2 \mathbf{R}}{\partial^2 \mathbf{v}} + {}^2\gamma \cdot \frac{\partial^2 \mathbf{H}}{\partial^2 \mathbf{v}} + {}^3\lambda \cdot \frac{\partial^3 \mathbf{R}}{\partial^2 \mathbf{v}} + {}^3\gamma \cdot \frac{\partial^3 \mathbf{H}}{\partial^2 \mathbf{v}} \right] \frac{D^2 \mathbf{v}}{D\phi_i} \\
 &\dots \\
 \left(\frac{D^{M-1} \hat{F}_I}{D\phi_i} \right)_{\lambda} &\equiv - \left[{}^{M-1}\lambda \cdot \frac{\partial^{M-1} \mathbf{R}}{\partial^{M-1} \mathbf{u}} + {}^{M-1}\gamma \cdot \frac{\partial^{M-1} \mathbf{H}}{\partial^{M-1} \mathbf{u}} + M\lambda \cdot \frac{\partial^M \mathbf{R}}{\partial^{M-1} \mathbf{u}} \right. \\
 &\quad \left. + M\gamma \cdot \frac{\partial^M \mathbf{H}}{\partial^{M-1} \mathbf{u}} \right] \frac{D^{M-1} \mathbf{u}}{D\phi_i} \\
 \left(\frac{D^{M-1} \hat{F}_I}{D\phi_i} \right)_{\gamma} &\equiv - \left[{}^{M-1}\lambda \cdot \frac{\partial^{M-1} \mathbf{R}}{\partial^{M-1} \mathbf{v}} + {}^{M-1}\gamma \cdot \frac{\partial^{M-1} \mathbf{H}}{\partial^{M-1} \mathbf{v}} + M\lambda \cdot \frac{\partial^M \mathbf{R}}{\partial^{M-1} \mathbf{v}} \right. \\
 &\quad \left. + M\gamma \cdot \frac{\partial^M \mathbf{H}}{\partial^{M-1} \mathbf{v}} \right] \frac{D^{M-1} \mathbf{v}}{D\phi_i} \\
 \left(\frac{D^M \hat{F}_I}{D\phi_i} \right)_{\lambda} &\equiv - \left[M\lambda \cdot \frac{\partial^M \mathbf{R}}{\partial^M \mathbf{u}} + M\gamma \cdot \frac{\partial^M \mathbf{H}}{\partial^M \mathbf{u}} - \frac{\partial^M \mathbf{G}}{\partial^M \mathbf{u}} \right] \frac{D^M \mathbf{u}}{D\phi_i} \\
 \left(\frac{D^M \hat{F}_I}{D\phi_i} \right)_{\gamma} &\equiv - \left[M\lambda \cdot \frac{\partial^M \mathbf{R}}{\partial^M \mathbf{v}} + M\gamma \cdot \frac{\partial^M \mathbf{H}}{\partial^M \mathbf{v}} - \frac{\partial^M \mathbf{G}}{\partial^M \mathbf{v}} \right] \frac{D^M \mathbf{v}}{D\phi_i}
 \end{aligned} \tag{74}$$

The above yields the following adjoint problems for ${}^n\lambda$ and ${}^n\gamma$, $n = 1, \dots, M$:

$$\begin{aligned}
 M : & \left\{ \begin{aligned} & \left[\frac{\partial {}^M\mathbf{R}}{\partial {}^M\mathbf{u}} - \frac{\partial {}^M\mathbf{R}}{\partial {}^M\mathbf{v}} \left(\frac{\partial {}^M\mathbf{H}}{\partial {}^M\mathbf{v}} \right)^{-1} \frac{\partial {}^M\mathbf{H}}{\partial {}^M\mathbf{u}} \right]^T {}^M\lambda = - \\ & \left[\left(\frac{\partial {}^M\mathbf{H}}{\partial {}^M\mathbf{v}} \right)^{-1} \frac{\partial {}^M\mathbf{H}}{\partial {}^M\mathbf{u}} \right]^T \frac{\partial G}{\partial {}^M\mathbf{v}} + \frac{\partial G}{\partial {}^M\mathbf{u}} \\ & {}^M\gamma = - \left(\frac{\partial {}^M\mathbf{H}}{\partial {}^M\mathbf{v}} \right)^{-T} \left[\left(\frac{\partial {}^M\mathbf{R}}{\partial {}^M\mathbf{v}} \right)^T {}^M\lambda - \frac{\partial G}{\partial {}^M\mathbf{v}} \right] \end{aligned} \right. \\
 M-1 : & \left\{ \begin{aligned} & \left[\frac{\partial {}^{M-1}\mathbf{R}}{\partial {}^{M-1}\mathbf{u}} - \frac{\partial {}^{M-1}\mathbf{R}}{\partial {}^{M-1}\mathbf{v}} \left(\frac{\partial {}^{M-1}\mathbf{H}}{\partial {}^{M-1}\mathbf{v}} \right)^{-1} \frac{\partial {}^{M-1}\mathbf{H}}{\partial {}^{M-1}\mathbf{u}} \right]^T {}^{M-1}\lambda = - \\ & \left[\frac{\partial {}^M\mathbf{R}}{\partial {}^{M-1}\mathbf{u}} - \frac{\partial {}^M\mathbf{R}}{\partial {}^{M-1}\mathbf{v}} \left(\frac{\partial {}^{M-1}\mathbf{H}}{\partial {}^{M-1}\mathbf{v}} \right)^{-1} \frac{\partial {}^{M-1}\mathbf{H}}{\partial {}^{M-1}\mathbf{u}} \right]^T {}^M\lambda - \\ & \left[\frac{\partial {}^M\mathbf{H}}{\partial {}^{M-1}\mathbf{u}} - \frac{\partial {}^M\mathbf{H}}{\partial {}^{M-1}\mathbf{v}} \left(\frac{\partial {}^{M-1}\mathbf{H}}{\partial {}^{M-1}\mathbf{v}} \right)^{-1} \frac{\partial {}^{M-1}\mathbf{H}}{\partial {}^{M-1}\mathbf{u}} \right]^T {}^M\gamma \\ & {}^{M-1}\gamma = - \left(\frac{\partial {}^{M-1}\mathbf{H}}{\partial {}^{M-1}\mathbf{v}} \right)^{-T} \left[\left(\frac{\partial {}^{M-1}\mathbf{R}}{\partial {}^{M-1}\mathbf{v}} \right)^T {}^{M-1}\lambda + \right. \\ & \quad \left. \left(\frac{\partial {}^M\mathbf{R}}{\partial {}^{M-1}\mathbf{v}} \right)^T {}^M\lambda + \left(\frac{\partial {}^M\mathbf{H}}{\partial {}^{M-1}\mathbf{v}} \right)^T {}^M\gamma \right] \end{aligned} \right. \\
 \dots & \\
 2 : & \left\{ \begin{aligned} & \left[\frac{\partial {}^2\mathbf{R}}{\partial {}^2\mathbf{u}} - \frac{\partial {}^2\mathbf{R}}{\partial {}^2\mathbf{v}} \left(\frac{\partial {}^2\mathbf{H}}{\partial {}^2\mathbf{v}} \right)^{-1} \frac{\partial {}^2\mathbf{H}}{\partial {}^2\mathbf{u}} \right]^T {}^2\lambda = - \\ & \left[\frac{\partial {}^3\mathbf{R}}{\partial {}^2\mathbf{u}} - \frac{\partial {}^3\mathbf{R}}{\partial {}^2\mathbf{v}} \left(\frac{\partial {}^2\mathbf{H}}{\partial {}^2\mathbf{v}} \right)^{-1} \frac{\partial {}^2\mathbf{H}}{\partial {}^2\mathbf{u}} \right]^T {}^3\lambda - \left[\frac{\partial {}^3\mathbf{H}}{\partial {}^2\mathbf{u}} - \frac{\partial {}^3\mathbf{H}}{\partial {}^2\mathbf{v}} \left(\frac{\partial {}^2\mathbf{H}}{\partial {}^2\mathbf{v}} \right)^{-1} \frac{\partial {}^2\mathbf{H}}{\partial {}^2\mathbf{u}} \right]^T {}^3\gamma \\ & {}^2\gamma = - \left(\frac{\partial {}^2\mathbf{H}}{\partial {}^2\mathbf{v}} \right)^{-T} \left[\left(\frac{\partial {}^2\mathbf{R}}{\partial {}^2\mathbf{v}} \right)^T {}^2\lambda + \left(\frac{\partial {}^3\mathbf{R}}{\partial {}^2\mathbf{v}} \right)^T {}^3\lambda + \left(\frac{\partial {}^3\mathbf{H}}{\partial {}^2\mathbf{v}} \right)^T {}^3\gamma \right] \end{aligned} \right. \\
 1 : & \left\{ \begin{aligned} & \left[\frac{\partial {}^1\mathbf{R}}{\partial {}^1\mathbf{u}} - \frac{\partial {}^1\mathbf{R}}{\partial {}^1\mathbf{v}} \left(\frac{\partial {}^1\mathbf{H}}{\partial {}^1\mathbf{v}} \right)^{-1} \frac{\partial {}^1\mathbf{H}}{\partial {}^1\mathbf{u}} \right]^T {}^1\lambda = - \\ & \left[\frac{\partial {}^2\mathbf{R}}{\partial {}^1\mathbf{u}} - \frac{\partial {}^2\mathbf{R}}{\partial {}^1\mathbf{v}} \left(\frac{\partial {}^1\mathbf{H}}{\partial {}^1\mathbf{v}} \right)^{-1} \frac{\partial {}^1\mathbf{H}}{\partial {}^1\mathbf{u}} \right]^T {}^2\lambda - \left[\frac{\partial {}^2\mathbf{H}}{\partial {}^1\mathbf{u}} - \frac{\partial {}^2\mathbf{H}}{\partial {}^1\mathbf{v}} \left(\frac{\partial {}^1\mathbf{H}}{\partial {}^1\mathbf{v}} \right)^{-1} \frac{\partial {}^1\mathbf{H}}{\partial {}^1\mathbf{u}} \right]^T {}^2\gamma \\ & {}^1\gamma = - \left(\frac{\partial {}^1\mathbf{H}}{\partial {}^1\mathbf{v}} \right)^{-T} \left[\left(\frac{\partial {}^1\mathbf{R}}{\partial {}^1\mathbf{v}} \right)^T {}^1\lambda + \left(\frac{\partial {}^2\mathbf{R}}{\partial {}^1\mathbf{v}} \right)^T {}^2\lambda + \left(\frac{\partial {}^2\mathbf{H}}{\partial {}^1\mathbf{v}} \right)^T {}^2\gamma \right] \end{aligned} \right. \quad (75)
 \end{aligned}$$

Again the operators for the adjoint problems are the transposes of the independent and dependent Newton-Raphson tangent operators used for the primal analysis.

Upon solving for the adjoint responses from equations (75), the sensitivities are computed from the analytic sensitivity term (cf. equation (73)). The solution of the adjoint problems (cf. (75)) proceeds in a regressive manner as in the transient nonlinear adjoint sensitivity analysis discussed in section 2.2.2.

The adjoint method for transient coupled systems has the same computational advantages

and disadvantages discussed for the transient nonlinear system. It requires recomputation or storage of the tangent operators and system response which increases either computation expense or storage requirements.

3 Rate-Independent Elasto-plasticity

Primal and sensitivity analyses of systems that exhibit history-dependent material response may be obtained directly from the previously discussed analyses of transient nonlinear coupled systems. To exemplify the proceeding analyses, rate-independent elasto-plasticity is investigated. The equilibrium and constitutive relations form the independent and dependent residuals for the analyses. Sensitivity expressions are derived for a general response functional via both the direct differentiation and adjoint methods. Finally, a one-dimensional, single degree-of-freedom problem is studied to illustrate the analyses.

3.1 Primal Analysis

Here, the equilibrium and constitutive equations are uncoupled by applying the solution process presented in section 2.4 for transient coupled nonlinear systems. A spatial domain V is considered, with boundary A , comprised of two complementary subsurfaces $A_{\mathbf{u}}$ and $A_{\mathbf{t}}$, with prescribed displacement and traction, respectively. A numerical solution is obtained by discretizing the time domain into M intervals and incorporating the backward Euler time integration scheme. Quasi-static loading is assumed, and therefore inertia effects are neglected.

The equilibrium condition is enforced at each time step n , i.e.

$$\nabla \cdot \mathbf{t} + \mathbf{b} = \mathbf{0} \quad \text{in } V \quad (76)$$

where \mathbf{t} and \mathbf{b} are the stress tensor and body force fields, respectively.

Infinitesimal deformations are assumed so that the strain-displacement relation reduces to

$${}^n \boldsymbol{\varepsilon}({}^n \mathbf{u}) = \frac{1}{2} [\nabla \cdot {}^n \mathbf{u} + (\nabla \cdot {}^n \mathbf{u})^T] \quad (77)$$

where \mathbf{u} is the displacement vector field and ∇ is the spatial gradient operator. Furthermore, the total strain tensor $\boldsymbol{\varepsilon}$ is expressed as a sum of its elastic part $\boldsymbol{\varepsilon}_E$ and plastic part $\boldsymbol{\varepsilon}_p$, as

$${}^n \boldsymbol{\varepsilon} = {}^n \boldsymbol{\varepsilon}_E + {}^n \boldsymbol{\varepsilon}_p \quad (78)$$

The constitutive relations consist of the plastic strain and internal variable evolution laws and the stress response, which are shown here in both their continuous and discrete

versions⁷, i.e.

$$\begin{aligned} {}^n\boldsymbol{\varepsilon}_p &= {}^{n-1}\boldsymbol{\varepsilon}_p + \int_{n-1}^n \dot{\boldsymbol{\varepsilon}}_p dt && \text{in } V \\ &\approx {}^{n-1}\boldsymbol{\varepsilon}_p + ({}^n\lambda - {}^{n-1}\lambda) \mathbf{f}({}^n\boldsymbol{\tau}, {}^n\mathbf{p}) && \text{in } V \end{aligned} \quad (79)$$

$$\begin{aligned} {}^n\mathbf{p} &= {}^{n-1}\mathbf{p} + \int_{n-1}^n \dot{\mathbf{p}} dt && \text{in } V \\ &\approx {}^{n-1}\mathbf{p} + ({}^n\lambda - {}^{n-1}\lambda) \mathbf{h}({}^n\boldsymbol{\tau}, {}^n\mathbf{p}) && \text{in } V \end{aligned} \quad (80)$$

$$\begin{aligned} {}^n\boldsymbol{\tau} &= {}^{n-1}\boldsymbol{\tau} + \mathbf{C} \left[\boldsymbol{\varepsilon}({}^n\mathbf{u}) - \boldsymbol{\varepsilon}({}^{n-1}\mathbf{u}) - \int_{n-1}^n \dot{\boldsymbol{\varepsilon}}_p dt \right] && \text{in } V \\ &\approx {}^{n-1}\boldsymbol{\tau} + \mathbf{C} \left[\boldsymbol{\varepsilon}({}^n\mathbf{u}) - \boldsymbol{\varepsilon}({}^{n-1}\mathbf{u}) - {}^n\boldsymbol{\varepsilon}_p + {}^{n-1}\boldsymbol{\varepsilon}_p \right] && \text{in } V \end{aligned} \quad (81)$$

where λ is the plastic multiplier, \mathbf{f} is the plastic flow vector, \mathbf{p} is the m -dimensional internal variable vector whose components describe internal dissipation mechanisms, \mathbf{h} is the hardening relation vector that governs the evolution law of \mathbf{p} , and \mathbf{C} is the elastic constitutive tensor.

The Kuhn-Tucker complementary conditions determine whether elastic behavior, loading, neutral loading or unloading occurs and are given in continuous and discrete form by

$$\begin{aligned} 0 &\leq \dot{\lambda} && \text{in } V \\ 0 &\leq {}^n\lambda - {}^{n-1}\lambda && \text{in } V \end{aligned} \quad (82)$$

$$\begin{aligned} 0 &\geq Y(\boldsymbol{\tau}, \mathbf{p}) && \text{in } V \\ 0 &\geq Y({}^n\boldsymbol{\tau}, {}^n\mathbf{p}) && \text{in } V \end{aligned} \quad (83)$$

$$\begin{aligned} 0 &= \dot{\lambda} Y(\boldsymbol{\tau}, \mathbf{p}) && \text{in } V \\ 0 &= ({}^n\lambda - {}^{n-1}\lambda) Y({}^n\boldsymbol{\tau}, {}^n\mathbf{p}) && \text{in } V \end{aligned} \quad (84)$$

where Y is the yield function.

The boundary conditions are

$$\begin{aligned} {}^n\mathbf{u} &= {}^n\mathbf{u}^P && \text{on } A_u \\ {}^n\mathbf{t} &= {}^n\mathbf{t}^P && \text{on } A_t \end{aligned} \quad (85)$$

where \mathbf{t} is the traction vector which is related to the stress tensor $\boldsymbol{\tau}$, through the Cauchy relation

$$\mathbf{t} = \boldsymbol{\tau} \cdot \mathbf{n} \quad \text{on } A \quad (86)$$

⁷Henceforth, vector notation [43] is used to represent the stress and strain tensor fields.

Here, \mathbf{n} is the unit outward normal to the surface A . For a detailed presentation of plasticity theory see [44, 45, 46].

The principle of virtual work yields the following variational form for the governing equation:

$$\int_V \boldsymbol{\varepsilon}(\hat{\mathbf{u}})^n \boldsymbol{\tau} dV = \int_V \hat{\mathbf{u}}^n \mathbf{b} dV + \int_{A_t} \hat{\mathbf{u}}^n \mathbf{t}^P dA \quad (87)$$

where $\hat{\mathbf{u}}$ is any kinematically admissible displacement field.

The transient coupled nonlinear system of equations (77) - (87) is solved with the finite element method by discretizing the spatial domain V , and introducing Gaussian quadratures to evaluate all spatial integrals in equation (77). Then, the Newton-Raphson iteration-subiteration process of section 2.4 is performed. The independent residual vector (cf. equation (63)) is formed from equation (87) by assembling the element residual vectors which in turn are evaluated by summing over the Gauss points [47], i.e.

$${}^n \mathbf{R} = \sum_{\text{elements}} \left(\sum_{\text{Gauss points}} {}^n \tilde{\mathbf{R}} \right) \quad (88)$$

where $(\tilde{\cdot})$ denotes quantities evaluated at the Gauss points. Here, ${}^n \mathbf{R} = \mathbf{0}$ is solved at the global level by performing the summations of equation (88). However, ${}^n \mathbf{H} = \mathbf{0}$ will be solved at the local level, i.e. at the Gauss point. Therefore, we have many ${}^n \mathbf{H}$ problems, one at each Gauss point in the mesh. In essence, in the primal analysis, we minimize ${}^n \mathbf{R}$ by averaging over the elements via the Galerkin method, whereas we minimize ${}^n \mathbf{H}$ at discrete points in the mesh via the collocation method. For this reason only Gauss point quantities are discussed in the remainder of this section.

For each element Gauss point, the residual ${}^n \tilde{\mathbf{R}}$ is expressed⁸ as

$${}^n \mathbf{R}({}^n \mathbf{U}, {}^{n-1} \mathbf{U}, {}^n \mathbf{v}, {}^{n-1} \mathbf{v}) = \mathbf{B}^T {}^n \boldsymbol{\tau} wJ - \mathbf{N}^T {}^n \mathbf{b} wJ - \mathbf{N}^T {}^n \mathbf{t} wj \quad (89)$$

where ${}^n \mathbf{U}$ is the N -degree-of-freedom element nodal displacement vector and \mathbf{N} and \mathbf{B} are the usual matrices which, when combined with ${}^n \mathbf{U}$, interpolate the displacement and strain, respectively, at the element Gauss points. Finally, J and j are the volume and area metrics and w is the weighting function.

The array ${}^n \mathbf{v}$, is defined at each Gauss point and is comprised of the plastic strain, internal variable vector, stress and plastic multiplier response fields, i.e.

$${}^n \mathbf{v} = \begin{bmatrix} {}^n \boldsymbol{\varepsilon}_p \\ {}^n \mathbf{p} \\ {}^n \boldsymbol{\tau} \\ {}^n \lambda \end{bmatrix} \quad (90)$$

⁸Henceforth, the $(\tilde{\cdot})$ is dropped with the understanding that all quantities are either evaluated or defined at the element Gauss point with the exception of the nodal quantities ${}^n \mathbf{U}$ and ${}^{n-1} \mathbf{U}$.

If elastic behavior or unloading occurs, then ${}^n\mathbf{v}$ reduces to ${}^n\mathbf{v} = [{}^n\boldsymbol{\tau}]$ and the dependent residual ${}^n\mathbf{H}$ is formed from equation (81), i.e.

$${}^n\mathbf{H} = {}^{n-1}\boldsymbol{\tau} + \mathbf{C} [\mathbf{B} {}^n\mathbf{U} - \mathbf{B} {}^{n-1}\mathbf{U}] - {}^n\boldsymbol{\tau} = \mathbf{0} \quad (91)$$

The above linear equation is trivially solved for ${}^n\boldsymbol{\tau}$. However, if neutral loading or plastic loading occurs, equations (79), (80), (81) and (84) are used to form the dependent residual ${}^n\mathbf{H}$ for the Gauss point,

$${}^n\mathbf{H}({}^n\mathbf{U}, {}^{n-1}\mathbf{U}, {}^n\mathbf{v}, {}^{n-1}\mathbf{v}) = \begin{bmatrix} {}^n\mathbf{H}_{\boldsymbol{\varepsilon}_p} \\ {}^n\mathbf{H}_{\mathbf{p}} \\ {}^n\mathbf{H}_{\boldsymbol{\tau}} \\ {}^nH_{\lambda} \end{bmatrix} = \mathbf{0} \quad (92)$$

where

$${}^n\mathbf{H}_{\boldsymbol{\varepsilon}_p} = {}^{n-1}\boldsymbol{\varepsilon}_p + ({}^n\lambda - {}^{n-1}\lambda) \mathbf{f}({}^n\boldsymbol{\tau}, {}^n\mathbf{p}) - {}^n\boldsymbol{\varepsilon}_p \quad (93)$$

$${}^n\mathbf{H}_{\mathbf{p}} = {}^{n-1}\mathbf{p} + ({}^n\lambda - {}^{n-1}\lambda) \mathbf{h}({}^n\boldsymbol{\tau}, {}^n\mathbf{p}) - {}^n\mathbf{p} \quad (94)$$

$${}^n\mathbf{H}_{\boldsymbol{\tau}} = {}^{n-1}\boldsymbol{\tau} + \mathbf{C} [\mathbf{B} {}^n\mathbf{U} - \mathbf{B} {}^{n-1}\mathbf{U} - {}^n\boldsymbol{\varepsilon}_p + {}^{n-1}\boldsymbol{\varepsilon}_p] - {}^n\boldsymbol{\tau} \quad (95)$$

$${}^nH_{\lambda} = Y({}^n\boldsymbol{\tau}, {}^n\mathbf{p}) \quad (96)$$

The independent tangent operator (cf. equation (41)) is computed in a manner analogous to the independent residual (cf. equation (88)), i.e.

$$\sum_{\text{elements}} \left(\sum_{\text{Gauss points}} \left[\frac{\partial {}^n\mathbf{R}}{\partial {}^n\mathbf{U}} - \frac{\partial {}^n\mathbf{R}}{\partial {}^n\mathbf{v}} \left(\frac{\partial {}^n\mathbf{H}}{\partial {}^n\mathbf{v}} \right)^{-1} \frac{\partial {}^n\mathbf{H}}{\partial {}^n\mathbf{U}} \right] \right) \quad (97)$$

where

$$\frac{\partial {}^n\mathbf{R}}{\partial {}^n\mathbf{U}} = \mathbf{0}_{N \times N} \quad (98)$$

$$\frac{\partial {}^n\mathbf{R}}{\partial {}^n\mathbf{v}} = \begin{bmatrix} \mathbf{0}_{N \times 6} & \mathbf{0}_{N \times m} & \mathbf{B}^T wJ & \mathbf{0}_{N \times 1} \end{bmatrix} \quad (99)$$

$$\frac{\partial {}^n\mathbf{H}}{\partial {}^n\mathbf{U}} = \begin{bmatrix} \mathbf{0}_{6 \times N} \\ \mathbf{0}_{m \times N} \\ \mathbf{CB} \\ \mathbf{0}_{1 \times N} \end{bmatrix} \quad (100)$$

and

$$\frac{\partial {}^n\mathbf{H}}{\partial {}^n\mathbf{v}} = \begin{bmatrix} \frac{\partial {}^n\mathbf{H}_{\boldsymbol{\varepsilon}_p}}{\partial {}^n\boldsymbol{\varepsilon}_p} & \frac{\partial {}^n\mathbf{H}_{\boldsymbol{\varepsilon}_p}}{\partial {}^n\mathbf{p}} & \frac{\partial {}^n\mathbf{H}_{\boldsymbol{\varepsilon}_p}}{\partial {}^n\boldsymbol{\tau}} & \frac{\partial {}^n\mathbf{H}_{\boldsymbol{\varepsilon}_p}}{\partial {}^n\lambda} \\ \frac{\partial {}^n\mathbf{H}_{\mathbf{p}}}{\partial {}^n\boldsymbol{\varepsilon}_p} & \frac{\partial {}^n\mathbf{H}_{\mathbf{p}}}{\partial {}^n\mathbf{p}} & \frac{\partial {}^n\mathbf{H}_{\mathbf{p}}}{\partial {}^n\boldsymbol{\tau}} & \frac{\partial {}^n\mathbf{H}_{\mathbf{p}}}{\partial {}^n\lambda} \\ \frac{\partial {}^n\mathbf{H}_{\boldsymbol{\tau}}}{\partial {}^n\boldsymbol{\varepsilon}_p} & \frac{\partial {}^n\mathbf{H}_{\boldsymbol{\tau}}}{\partial {}^n\mathbf{p}} & \frac{\partial {}^n\mathbf{H}_{\boldsymbol{\tau}}}{\partial {}^n\boldsymbol{\tau}} & \frac{\partial {}^n\mathbf{H}_{\boldsymbol{\tau}}}{\partial {}^n\lambda} \\ \frac{\partial {}^nH_{\lambda}}{\partial {}^n\boldsymbol{\varepsilon}_p} & \frac{\partial {}^nH_{\lambda}}{\partial {}^n\mathbf{p}} & \frac{\partial {}^nH_{\lambda}}{\partial {}^n\boldsymbol{\tau}} & \frac{\partial {}^nH_{\lambda}}{\partial {}^n\lambda} \end{bmatrix}$$

$$= \begin{bmatrix} -\mathbf{I}_{6 \times 6} & ({}^n\lambda - {}^{n-1}\lambda) \frac{\partial \mathbf{f}}{\partial {}^n\mathbf{p}} & ({}^n\lambda - {}^{n-1}\lambda) \frac{\partial \mathbf{f}}{\partial {}^n\mathcal{T}} & \mathbf{f} \\ \mathbf{0}_{m \times 6} & ({}^n\lambda - {}^{n-1}\lambda) \frac{\partial \mathbf{h}}{\partial {}^n\mathbf{p}} - \mathbf{I}_{m \times m} & ({}^n\lambda - {}^{n-1}\lambda) \frac{\partial \mathbf{h}}{\partial {}^n\mathcal{T}} & \mathbf{h} \\ -\mathbf{C} & \mathbf{0}_{6 \times m} & -\mathbf{I}_{6 \times 6} & \mathbf{0}_{6 \times 1} \\ \mathbf{0}_{1 \times 6} & \frac{\partial Y}{\partial {}^n\mathbf{p}} & \frac{\partial Y}{\partial {}^n\mathcal{T}} & 0 \end{bmatrix} \quad (101)$$

It is emphasized here that equations (89) and (97) cannot be evaluated until the local residual problem ${}^n\mathbf{H} = \mathbf{0}$ is solved at the Gauss point to first determine ${}^n\mathbf{v}({}^n\mathbf{U}^I)$ and $\frac{D}{}^n\mathbf{U}}{D}({}^n\mathbf{U}^I)$. After the summations of equation (97) are evaluated, the independent tangent stiffness is used in equation (41) to evaluate $\delta\mathbf{U}$. Note that this analysis is entirely equivalent to the analytical consistent tangent operator approach in [36] and the numerical approach in [42].

3.2 Sensitivity Analysis

Both the direct differentiation and adjoint methods are presented for the sensitivity analysis (cf. sections 2.4.1 and 2.4.2). The computation of the pseudo and adjoint load vectors and evaluation of the pseudo or adjoint response, respectively is first discussed. Then, the explicit derivative quantities are addressed.

In the direct differentiation method, the independent pseudo loads (cf. equation (70)), are formed by assembling the element pseudo load vectors which are evaluated by summing over the Gauss points, in a manner analogous to the formation of the independent residual (cf. equation (88)). Upon evaluating the derivative $\frac{\partial {}^n\mathbf{U}}{\partial \phi_i}$, via a back substitution using the previously decomposed independent tangent stiffness matrix, the derivative $\frac{\partial {}^n\mathbf{v}}{\partial \phi_i}$ is computed at each Gauss point by forming the dependent pseudo loads (cf. equation (69)) followed by a back substitution using the previously decomposed dependent tangent stiffness matrices.

In the adjoint method, the independent adjoint response ${}^n\boldsymbol{\lambda}$ is computed by forming the independent adjoint load vector (cf. equation (75)) followed by a back substitution using the transpose of the previously decomposed independent tangent operator. Next, the dependent adjoint response ${}^n\boldsymbol{\gamma}$ is evaluated at each Gauss point (cf. equation (75)) by forming the dependent adjoint load followed by a back substitution using the transpose of the previously decomposed dependent tangent operator.

The operators $\frac{\partial {}^n\mathbf{R}}{\partial {}^{n-1}\mathbf{U}}$, $\frac{\partial {}^n\mathbf{R}}{\partial {}^{n-1}\mathbf{v}}$, $\frac{\partial {}^n\mathbf{H}}{\partial {}^{n-1}\mathbf{U}}$, and $\frac{\partial {}^n\mathbf{H}}{\partial {}^{n-1}\mathbf{v}}$ for each Gauss point are computed as

$$\frac{\partial {}^n\mathbf{R}}{\partial {}^{n-1}\mathbf{U}} = \mathbf{0}_{N \times N} \quad (102)$$

$$\frac{\partial^n \mathbf{R}}{\partial^{n-1} \mathbf{v}} = \mathbf{0}_{N \times (6+m+6+1)} \quad (103)$$

$$\frac{\partial^n \mathbf{H}}{\partial^{n-1} \mathbf{U}} = \begin{bmatrix} \mathbf{0}_{6 \times N} \\ \mathbf{0}_{m \times N} \\ \mathbf{CB} \\ \mathbf{0}_{1 \times N} \end{bmatrix} \quad (104)$$

$$\frac{\partial^n \mathbf{H}}{\partial^{n-1} \mathbf{v}} = \begin{bmatrix} \mathbf{I}_{6 \times 6} & \mathbf{0}_{6 \times m} & \mathbf{0}_{6 \times 6} & -\mathbf{f} \\ \mathbf{0}_{m \times 6} & \mathbf{I}_{m \times m} & \mathbf{0}_{m \times 6} & -\mathbf{h} \\ \mathbf{C} & \mathbf{0}_{6 \times m} & \mathbf{I}_{6 \times 6} & \mathbf{0}_{6 \times 1} \\ \mathbf{0}_{1 \times 6} & \mathbf{0}_{1 \times m} & \mathbf{0}_{1 \times 6} & 0 \end{bmatrix} \quad (105)$$

The quantities $\frac{\partial G}{\partial \mathbf{u}}$, $\frac{\partial G}{\partial \mathbf{v}}$, $\frac{\partial G}{\partial \mathbf{u}}$, $\frac{\partial G}{\partial \mathbf{v}}$, $\frac{\partial G}{\partial \phi_i}$, $\frac{\partial^n \mathbf{R}}{\partial \phi_i}$ and $\frac{\partial^n \mathbf{H}}{\partial \phi_i}$ depend on the choice of the response functional G , and the parameterization ϕ . For a general case, see [34]. In the following example, a few possibilities are presented.

3.2.1 Existence Issues in Sensitivity Analysis

It is well known that the existence of sensitivities is not always guaranteed. For example, problems with repeated eigenvalues have only directional derivatives (cf. [3]). The plasticity problem is also prone to the nonexistence issue when design changes result in transitions from elastic to plastic material behavior and vice-versa. In this transitional case, only directional sensitivities exist. For example, at a given material point, a positive design change may induce plastic behavior while a negative change may induce elastic behavior. Non-existence issues are present in continuous formulations for all points which just contact the yield surface, i.e. those points for which neutral loading occurs, where $\dot{\lambda}$ and Y are equal to zero in equation (84). However, in finite element applications, the elastic-plastic transition is monitored only at the Gauss points so that these neutral loading points are less apt to be encountered. Furthermore, due to the numerical precision, it is extremely unlikely that the condition $\dot{\lambda}$ and Y equal to zero will be exactly satisfied. Rather, the majority of the Gauss points which undergo a transition from the elastic to plastic regions in a given load step are placed well into the plastic regime. Therefore, design perturbations, whether positive or negative, will still result in plastic behavior at the Gauss point, so the Frechet derivative exists, i.e. there is no need to consider directional derivatives for the numerical computations.

Directional derivatives have been used in sensitivity analyses to monitor the transition points in simple structures [28, 29]. However, this approach is not practical for large systems

as it places severe restrictions on the load step size. Furthermore, our numerical experience has shown that special treatment for transition points is not necessary to compute accurate sensitivities [34], again because so few points are precisely at the transition point. Finally, we note that these existence issues arise in all analyses which contain discontinuities but, for numerical computations are ignored. For example, accurate sensitivities are calculated for nonlinear conduction problems with piecewise linear conductivity material model, again without any special treatments of the transition points [20, 21].

3.3 Analytical Example

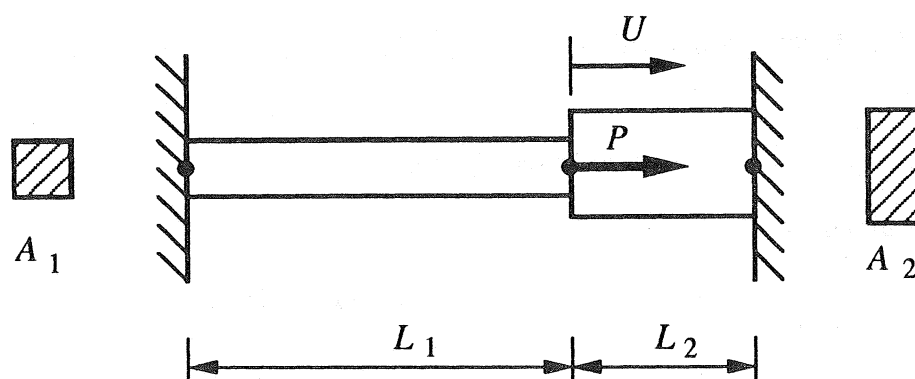


Figure 2: One-dimension single degree-of-freedom two bar system.

The one-dimension single degree-of-freedom system illustrated in figure 2 is studied to demonstrate the formation of the tangent operators and the design sensitivities for small deformation elasto-plasticity. The primal analysis for this example is presented in a continuous time domain in [48]. The two bars have lengths L_1 , L_2 and cross-sections A_1 , A_2 respectively, where $\frac{L_1}{L_2} = 2$ and $\frac{A_2}{A_1} = 2$. The bars are constrained at the edges and are connected at the mid-node where the axial load P , is applied. The mid-node axial displacement U comprises the single independent degree-of-freedom. Both bars consist of the same material with yield function

$$Y = \tau_p - (\tau_y + kEe_p) \quad (106)$$

Here, τ_y is the initial yield stress, E is the elastic modulus, k is a material coefficient ($k = 1/4$), and τ_p and $e_p = \int \dot{e}_p dt$ are the equivalent plastic stress and strain, respectively⁹

$$\tau_p \equiv \sqrt{\frac{3}{2} s_i s_i} \quad (107)$$

⁹Summation convention is enforced on repeated indices.

and

$$\dot{\epsilon}_p \equiv \sqrt{\frac{2}{3} \dot{\epsilon}_{p_i} \dot{\epsilon}_{p_i}} \quad (108)$$

where s_i are the deviatoric stress components

$$s_i \equiv \begin{cases} \tau_i - \frac{1}{3}(\tau_1 + \tau_2 + \tau_3) & , \text{ for } i = 1, 2, 3 \\ \tau_i & , \text{ for } i = 4, 5, 6 \end{cases} \quad (109)$$

From equation (106), the internal variable vector \mathbf{p} becomes

$$\mathbf{p} = [p_1] = [e_p] \quad (110)$$

The only non-zero stress component is τ_1 due to uniaxial behavior; therefore, the equivalent stress becomes

$$\tau_p = |\tau_1| = \text{sign}(\tau_1)\tau_1 \quad (111)$$

where sign is defined as

$$\text{sign}(\cdot) \equiv \begin{cases} + & , \text{ for } \cdot \geq 0 \\ - & , \text{ for } \cdot < 0 \end{cases} \quad (112)$$

By using associative plasticity, the flow vector is given by the normality rule

$$\mathbf{f} = \left[\frac{\partial Y}{\partial \boldsymbol{\tau}} \right]^T = \text{sign}(\tau_1) \begin{bmatrix} 1 \\ -\frac{1}{2} \\ -\frac{1}{2} \\ 0 \\ 0 \\ 0 \end{bmatrix} \quad (113)$$

Substitution of equation (113) into equation (79) yields $\epsilon_{p_2} = \epsilon_{p_3} = -\frac{1}{2}\epsilon_{p_1}$ and $\epsilon_{p_4} = \epsilon_{p_5} = \epsilon_{p_6} = 0$. Then, by using equations (79), (80), (108) and (113) the hardening vector \mathbf{h} , is given by

$$\mathbf{h} = [1] \quad (114)$$

The primary response quantities reduce to U and λ as well as q_1 , τ_1 and ϵ_{p_1} which will be denoted as q , τ and ϵ_p henceforth, for conciseness. All response fields are, at most, linear functions of the spatial variables so that a single point quadrature evaluates the spatial integrals of equation (87) exactly. For the center Gauss point and mid-node degree-of-freedom,

$$\mathbf{N} = \begin{bmatrix} 1 \\ 2 \end{bmatrix} \quad (115)$$

and

$$\mathbf{B} = \left[\pm \frac{1}{L} \right] \quad (116)$$

where the + and - in \pm above and henceforth refer to the left and right bar, respectively. The volume metric becomes $J = \frac{AL}{2}$ and the weight function becomes $w = 2$. The equilibrium residual ${}^n\mathbf{R}$ for the left bar is given by

$${}^n\mathbf{R} = [A_1 {}^n\tau] \quad (117)$$

and for the right bar it is given by

$${}^n\mathbf{R} = [-A_2 {}^n\tau - {}^nP] \quad (118)$$

If a bar is undergoing elastic deformation, the response vector ${}^n\mathbf{v}$ is comprised solely by the stress component ${}^n\tau$, i.e.

$${}^n\mathbf{v} = [{}^n\tau] \quad (119)$$

and the residual ${}^n\mathbf{H}$ becomes

$${}^n\mathbf{H} = \left[{}^{n-1}\tau \pm E \frac{{}^nU - {}^{n-1}U}{L} - {}^n\tau \right] \quad (120)$$

The operators $\frac{\partial {}^n\mathbf{R}}{\partial {}^n\mathbf{U}}$, $\frac{\partial {}^n\mathbf{R}}{\partial {}^n\mathbf{v}}$, $\frac{\partial {}^n\mathbf{H}}{\partial {}^n\mathbf{U}}$, $\frac{\partial {}^n\mathbf{H}}{\partial {}^n\mathbf{v}}$, and $\left(\frac{\partial {}^n\mathbf{H}}{\partial {}^n\mathbf{v}}\right)^{-1}$ become

$$\frac{\partial {}^n\mathbf{R}}{\partial {}^n\mathbf{U}} = [0] \quad (121)$$

$$\frac{\partial {}^n\mathbf{R}}{\partial {}^n\mathbf{v}} = [\pm A] \quad (122)$$

$$\frac{\partial {}^n\mathbf{H}}{\partial {}^n\mathbf{U}} = \left[\pm \frac{E}{L} \right] \quad (123)$$

$$\frac{\partial {}^n\mathbf{H}}{\partial {}^n\mathbf{v}} = [-1] \quad (124)$$

$$\left(\frac{\partial {}^n\mathbf{H}}{\partial {}^n\mathbf{v}}\right)^{-1} = [-1] \quad (125)$$

If a bar is undergoing plastic deformation, the response vector ${}^n\mathbf{v}$ and the residual ${}^n\mathbf{H}$ are given by equations (90) and (92), respectively, where

$${}^n\mathbf{H}_{\epsilon_p} = \left[{}^{n-1}\epsilon_p + \text{sign}(\tau_1)({}^n\lambda - {}^{n-1}\lambda) - {}^n\epsilon_p \right] \quad (126)$$

$${}^n\mathbf{H}_p = \left[{}^{n-1}p + ({}^n\lambda - {}^{n-1}\lambda) - {}^np \right] \quad (127)$$

$${}^n\mathbf{H}_{\tau} = \left[{}^{n-1}\tau + E \left(\pm \frac{{}^nU - {}^{n-1}U}{L} - {}^n\epsilon_p + {}^{n-1}\epsilon_p \right) - {}^n\tau \right] \quad (128)$$

$${}^nH_{\lambda} = \text{sign}(\tau_1) {}^n\tau - (\tau_y + kE {}^nq) \quad (129)$$

Then, the operators $\frac{\partial^n \mathbf{R}}{\partial^n \mathbf{U}}$, $\frac{\partial^n \mathbf{R}}{\partial^n \mathbf{v}}$, $\frac{\partial^n \mathbf{H}}{\partial^n \mathbf{U}}$, $\frac{\partial^n \mathbf{H}}{\partial^n \mathbf{v}}$, and $\left(\frac{\partial^n \mathbf{H}}{\partial^n \mathbf{v}}\right)^{-1}$ become

$$\frac{\partial^n \mathbf{R}}{\partial^n \mathbf{U}} = [0] \quad (130)$$

$$\frac{\partial^n \mathbf{R}}{\partial^n \mathbf{v}} = [0 \ 0 \ \pm A \ 0] \quad (131)$$

$$\frac{\partial^n \mathbf{H}}{\partial^n \mathbf{U}} = \begin{bmatrix} 0 \\ 0 \\ \pm \frac{E}{L} \\ 0 \end{bmatrix} \quad (132)$$

$$\frac{\partial^n \mathbf{H}}{\partial^n \mathbf{v}} = \begin{bmatrix} -1 & 0 & 0 & \text{sign}(\tau_1) \\ 0 & -1 & 0 & 1 \\ -E & 0 & -1 & 0 \\ 0 & -kE & \text{sign}(\tau_1) & 0 \end{bmatrix} \quad (133)$$

$$\left(\frac{\partial^n \mathbf{H}}{\partial^n \mathbf{v}}\right)^{-1} = \frac{1}{1+k} \begin{bmatrix} -k & \text{sign}(\tau_1)k & -\frac{1}{E} & -\text{sign}(\tau_1)\frac{1}{E} \\ \text{sign}(\tau_1) & -1 & -\text{sign}(\tau_1)\frac{1}{E} & -\frac{1}{E} \\ Ek & -\text{sign}(\tau_1)Ek & -k & \text{sign}(\tau_1) \\ \text{sign}(\tau_1) & k & -\text{sign}(\tau_1)\frac{1}{E} & -\frac{1}{E} \end{bmatrix} \quad (134)$$

Three load steps are applied, which successively induce initial plastification of the right bar, initial plastification of the left bar and further plastification of both bars. The results are denoted in table 1 and agree with those in [48].

$P/(A_1\tau_y)$	$UE/(\tau_y L_1)$	Left bar		Right bar	
		τ/τ_y	$\varepsilon_p E/\tau_y$	τ/τ_y	$\varepsilon_p E/\tau_y$
0	0	0	0	0	0
5/2	1/2	1/2	0	-1	0
17/5	1	1	0	-6/5	-4/5
4	8/5	28/25	12/25	-36/25	-44/25

Table 1: Primal analysis results

3.3.1 Sensitivity Analysis

The terminal mid-node displacement 3U is defined as the response functional F , i.e.

$$F(\phi) = G({}^3\mathbf{u}(\phi), \phi) = {}^3U(\phi) \quad (135)$$

and the initial yield stress τ_y is chosen as the single design parameter, i.e. $\phi = \tau_y$. Additionally the load P is defined as a function of the initial yield stress τ_y , i.e. ${}^1P = \frac{5}{2}A_1\tau_y$, ${}^2P = \frac{17}{5}A_1\tau_y$ and ${}^3P = 4A_1\tau_y$, to avoid the existence issues in the sensitivity analysis regarding transitions from the elastic and plastic regions (cf. section 3.2). Zero sensitivities for all initial conditions are assigned.

For the response functional considered, $\frac{\partial G}{\partial {}^3U} = 1$, $\frac{\partial G}{\partial {}^3\mathbf{v}} = \mathbf{0}$ and $\frac{\partial G}{\partial \phi} = 0$. The explicit sensitivity $\frac{\partial {}^n\mathbf{R}}{\partial \phi}$ for the left bar becomes

$$\frac{\partial {}^n\mathbf{R}}{\partial \phi} = [0] \quad (136)$$

and for the right bar,

$$\frac{\partial {}^1\mathbf{R}}{\partial \phi} = \left[\frac{5}{2}A_1 \right] \quad (137)$$

$$\frac{\partial {}^2\mathbf{R}}{\partial \phi} = \left[\frac{17}{5}A_1 \right] \quad (138)$$

$$\frac{\partial {}^3\mathbf{R}}{\partial \phi} = [4A_1] \quad (139)$$

For a bar with only elastic deformation, the explicit sensitivity $\frac{\partial {}^n\mathbf{H}}{\partial \phi}$ becomes

$$\frac{\partial {}^n\mathbf{H}}{\partial \phi} = [0] \quad (140)$$

and the operators $\frac{\partial {}^n\mathbf{R}}{\partial {}^{n-1}\mathbf{U}}$, $\frac{\partial {}^n\mathbf{R}}{\partial {}^{n-1}\mathbf{v}}$, $\frac{\partial {}^n\mathbf{H}}{\partial {}^{n-1}\mathbf{U}}$ and $\frac{\partial {}^n\mathbf{H}}{\partial {}^{n-1}\mathbf{v}}$, equal

$$\frac{\partial {}^n\mathbf{R}}{\partial {}^{n-1}\mathbf{U}} = [0] \quad (141)$$

$$\frac{\partial {}^n\mathbf{R}}{\partial {}^{n-1}\mathbf{v}} = [0] \quad (142)$$

$$\frac{\partial {}^n\mathbf{H}}{\partial {}^{n-1}\mathbf{U}} = \left[\mp \frac{E}{L} \right] \quad (143)$$

$$\frac{\partial {}^n\mathbf{H}}{\partial {}^{n-1}\mathbf{v}} = [1] \quad (144)$$

For a bar undergoing plastic deformation, the explicit sensitivity $\frac{\partial^n \mathbf{H}}{\partial \phi}$ becomes

$$\frac{\partial^n \mathbf{H}}{\partial \phi} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ -1 \end{bmatrix} \quad (145)$$

and the operators $\frac{\partial^n \mathbf{R}}{\partial^{n-1} \mathbf{U}}$, $\frac{\partial^n \mathbf{R}}{\partial^{n-1} \mathbf{v}}$, $\frac{\partial^n \mathbf{H}}{\partial^{n-1} \mathbf{U}}$, and $\frac{\partial^n \mathbf{H}}{\partial^{n-1} \mathbf{v}}$ equal

$$\frac{\partial^n \mathbf{R}}{\partial^{n-1} \mathbf{U}} = [0] \quad (146)$$

$$\frac{\partial^n \mathbf{R}}{\partial^{n-1} \mathbf{v}} = [0 \ 0 \ 0 \ 0] \quad (147)$$

$$\frac{\partial^n \mathbf{H}}{\partial^{n-1} \mathbf{U}} = \begin{bmatrix} 0 \\ 0 \\ \mp \frac{E}{L} \\ 0 \end{bmatrix} \quad (148)$$

$$\frac{\partial^n \mathbf{H}}{\partial^{n-1} \mathbf{v}} = \begin{bmatrix} 1 & 0 & 0 & -\text{sign}(\tau_1) \\ 0 & 1 & 0 & -1 \\ E & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix} \quad (149)$$

Implementation of the direct differentiation method follows from section 2.4.1. First, the implicit derivatives $\frac{\partial^n U}{\partial \phi}$ and $\frac{\partial^n \mathbf{v}}{\partial \phi}$ are computed and then, the sensitivity $\frac{DF}{D\phi}$ is evaluated from equation (68). The computed values of the implicit derivatives are denoted in table 2. Substitution of $\frac{\partial^3 U}{\partial \phi}$ and $\frac{\partial^3 \mathbf{v}}{\partial \phi}$ into equation (68) yields $\frac{DF}{D\phi} = \frac{8}{5} \frac{L_1}{E}$ for the sensitivity. This sensitivity value equals that obtained by differentiating the analytical result ${}^3U = \frac{8}{5} \frac{L_1 \tau_y}{E}$ (cf. table 1).

The sensitivity is also computed with the adjoint method (cf. section 2.4.2). The terminal adjoint problem is solved for the adjoint responses ${}^n \boldsymbol{\lambda}$ and ${}^n \boldsymbol{\gamma}$ (cf. equation (75)), and the sensitivity is computed from equation (73). The computed adjoint responses ${}^n \boldsymbol{\lambda}$ and ${}^n \boldsymbol{\gamma}$ are presented in table 3. As expected, the adjoint sensitivity is identical to the direct differentiation and analytical sensitivity results.

Time step n	$\frac{D^n U}{D\phi}$	Left bar	Right bar
		$\frac{D^n \mathbf{v}}{D\phi}$	
1	$\frac{1}{2} \frac{L_1}{E}$	$\begin{bmatrix} 1 \\ 2 \end{bmatrix}$	$[-1]$
2	$1 \frac{L_1}{E}$	$[1]$	$\begin{bmatrix} -\frac{4}{5} \frac{1}{E} \\ \frac{4}{5} \frac{1}{E} \\ -\frac{6}{5} \\ \frac{4}{5} \frac{1}{E} \end{bmatrix}$
3	$\frac{8}{5} \frac{L_1}{E}$	$\begin{bmatrix} \frac{12}{25} \frac{1}{E} \\ \frac{12}{25} \frac{1}{E} \\ \frac{28}{25} \\ \frac{12}{25} \frac{1}{E} \end{bmatrix}$	$\begin{bmatrix} -\frac{44}{25} \frac{1}{E} \\ \frac{44}{25} \frac{1}{E} \\ -\frac{36}{25} \\ \frac{44}{25} \frac{1}{E} \end{bmatrix}$

Table 2: Direct differentiation analysis results

Time step n	${}^n\lambda$	Left bar	Right bar
		${}^n\gamma$	
3	$\left[\frac{L_1}{A_1 E}\right]$	$\begin{bmatrix} -\frac{L_1}{5} \\ \frac{L_1}{5} \\ \frac{L_1}{5E} \\ -\frac{4L_1}{5E} \end{bmatrix}$	$\begin{bmatrix} \frac{2L_1}{5} \\ \frac{2L_1}{5} \\ -\frac{2L_1}{5E} \\ -\frac{8L_1}{5E} \end{bmatrix}$
2	$[0]$	$\left[\frac{L_1}{5E}\right]$	$\begin{bmatrix} \frac{2L_1}{5} \\ \frac{2L_1}{5} \\ -\frac{2L_1}{5E} \\ 0 \end{bmatrix}$
1	$[0]$	$\left[\frac{L_1}{5E}\right]$	$\left[-\frac{2L_1}{5E}\right]$

Table 3: Adjoint analysis results

4 Conclusion

A general approach for analysis and analytic design sensitivity analysis of transient coupled nonlinear problems is presented. The general approach is initially developed for steady-state uncoupled nonlinear systems, extended to transient uncoupled and steady-state coupled nonlinear systems, and finally derived for transient coupled nonlinear systems.

A systematic numerical procedure for constructing consistent tangent operators, which are necessary for a quadratically convergent solution algorithm, is discussed. This is an efficient alternative to the closed-form approach in [36], especially when complex constitutive relations are used. The necessity of the consistent tangent operator is also shown in regard to the evaluation of accurate sensitivities.

Both direct and adjoint sensitivity methods are discussed. A detailed description of an adjoint sensitivity method is presented for transient systems. The method requires the solution of an adjoint transient terminal-value problem. Since the definition of the adjoint terminal-value problem depends on the solution of the original initial-value problem, the sensitivity analysis cannot be performed simultaneously with the primal analysis. This complication increases either the computational expense or storage requirements. It appears, therefore, that the direct differentiation method is more suitable for transient systems. However, if the number of functionals for which design sensitivities are desired is much less than the number of design parameters, the adjoint approach may still be preferred.

The general framework for deriving tangent operators and analytic sensitivity expressions, discussed in section 2, is easily particularized to accommodate various problem classes. This versatility is demonstrated in section 3 by specializing the transient coupled formulation to rate-independent elasto-plasticity. A one-dimensional elasto-plastic example with an analytical solution is presented, where the sensitivities are evaluated by both the direct differentiation and adjoint methods.

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