ADJOINT SENSITIVITY ANALYSIS OF THE THERMOMECHANICAL BEHAVIOR OF REPOSITORIES

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ABSTRACT

The adjoint sensitivity method is applied to thermomechanical models for the first time. The method provides an efficient and inexpensive answer to the question: how sensitive are thermomechanical predictions to assumed parameters? The answer is exact, in the sense that it yields exact derivatives of response measures to parameters, and approximate, in the sense that projections of the response for other parameter assumptions are only first order correct. The method is applied to linear finite element models of thermomechanical behavior. Extensions to more complicated models are straight-forward but often laborious. An illustration of the method with a two-dimensional repository corridor model reveals that the chosen stress response measure was most sensitive to Poisson's ratio for the rock matrix.

INTRODUCTION

Computer simulation models developed to assess the thermomechanical behavior of repositories and the surrounding rock are subject to uncertainties. In some cases our understanding of constitutive relationships describing the behavior is still evolving. In almost all cases there is uncertainty about the material properties and other parameters assigned to the model. Parameter uncertainty is typically dealt with by using multiple simulation runs while varying the parameters in a systematic, or more often, an ad hoc way. This process is often refered to as sensitivity analysis. In this paper we introduce to thermomechanical models an efficient and systematic method of parameter sensitivity analysis. It is called 'adjoint sensitivity analysis'.

The method is well accepted mathematically and has been applied in optimal control[1,2], nonlinear estimation[3,4], and parameter sensitivity analysis[5,6,7]. We first introduce the method with a simple example, then apply it to a linear thermomechanical finite element model, and finally illustrate its use in a typical repository setting.

Response Measure and its Sensitivity

To determine parameter sensitivity we usually designate one or more measures of how the thermomechanical system is behaving. These measures may be as complicated as a description of the zone of rock which has yielded or perhaps failed, or may be as simple as a principal stress at a critical point. In this paper we assume that the measures selected are taken at fixed locations in space, can be represented by scalar numbers and are differentiable. More general measures involving, for example, the location of a critical point or the size of the zone of yield or failure, can be attacked analogously but are beyond the scope of this introductory presentation. We'll call a scalar measure of system behavior the 'response measure', although the term 'response function' or 'performance measure' can also be used, and denote it by the letter J. Examples of response measures that can be considered with these constraints are displacements at prescribed points, differential displacements between points, average displacement along a boundary, any strain or stress component at prescribed points, a principal strain or stress at prescribed points, and various yield criteria at prescribed points.

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SIMPLE EXAMPLE

We wish to determine the sensitivity of the response to assumed parameters, designated by the symbol u. Take the special case of a single parameter u, then by varying u and rerunning the model several times we would generate a response curve J(u) such as shown in Fig. 1. With more than

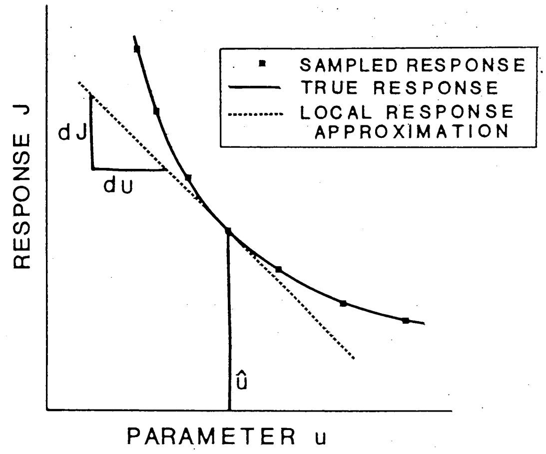

Fig. 1. Response curve J(u) for parameter u.

one parameter u the curve becomes a surface for which generation in practice becomes so expensive it is seldom found. Suppose that our best estimate of u is $\hat{u}$, then a measure of the sensitivity of the response J to u is the derivative of J at $\hat{u}$:

$$\text{sensitivity} = \left.\frac{dJ}{du}\right|_{u=\hat{u}} \tag{1}$$

In Fig. 1 this derivative is pictured as the straight line tangent to the response curve at $\hat{u}$, and provides a first order approximation to J(u) for $u \neq \hat{u}$:

$$J(u) \simeq J(\hat{u}) + (u-\hat{u}) \left.\frac{dJ}{du}\right|_{u=\hat{u}} \tag{2}$$

The derivative could be approximated by making two computer runs with $u = \hat{u} \pm \Delta u$, where Δu is a small perturbation of the parameter. In a system with many parameters this perturbation approach requires at least two runs for each parameter, or so many runs that even the calculation of sensitivity derivatives can become prohibitively expensive.

Another approach involves the recognition that the response function depends on parameters u both directly and indirectly, through the system state which we'll denote x in our simple example. In thermomechanical models temperatures and displacements are typical states. Thus, J = J[u,x(u)] and the sensitivity derivative in Eq. (1) can be expanded as:

$$\left.\frac{dJ}{du}\right|_{\hat{u}} = \left.\frac{\partial J}{\partial u}\right|_{\hat{u}} + \frac{\partial J}{\partial x}\left.\frac{\partial x}{\partial u}\right|_{\hat{u}} \tag{3}$$

The derivatives $\partial J/\partial u$, in which $x = x(\hat{u})$ is held constant, and $\partial J/\partial x$, in which $u = \hat{u}$ is held constant, can usually be easily found, but the state derivative $\partial x/\partial u$ requires a new solution of the system of equations for each parameter u of interest. To understand why this is so we must examine our original problem. Take it to be the simple state equation:

$$ax = b \tag{4}$$

where a and b are parameters. Then, assuming that Eq. (4) is differentiable, we can also write:

$$a\frac{\partial x}{\partial u} = \frac{\partial b}{\partial u} - \frac{\partial a}{\partial u}x \tag{5}$$

For every u we must solve an equation of this type. In the trivial example of Eq. (4) the solutions are $\partial x/\partial a = -b/a^2$ and $\partial x/\partial b = 1/a$, for u = a and b. In real problems with many parameters multiple computer runs solving Eq. (5) are required, although the resulting sensitivity derivatives in Eq. (3) are now exact and not simply the approximations that are found with the perturbation approach.

Simplified Adjoint Approach

The adjoint method avoids the use of repetitious computer runs by suggesting a new problem to be solved, one that is somewhat similar to our original problem yet directly involves a specific response measure. As a consequence there is one adjoint problem to be solved for each response measure selected. For our simple example, Eq. (4), and certain other problems the method can be derived as follows. Substitute Eq. (5) into Eq. (3) to yield:

$$\frac{dJ}{du} = \frac{\partial J}{\partial u} + \frac{\partial J}{\partial x}a^{-1}\left(\frac{\partial b}{\partial u} - \frac{\partial a}{\partial u}x\right) \tag{6}$$

Recognize that both $\partial J/\partial x$ and a^{-1} are known or can be easily found, so that their product is also known. Denote this product λ:

$$\lambda = \frac{\partial J}{\partial x}a^{-1} \tag{7}$$

or

$$a\lambda = \frac{\partial J}{\partial x} \tag{8}$$

Equation (8) is called the 'adjoint problem' and λ is said to be an 'adjoint state' or 'co-state'. Equation (8) has the same form as our original state equation, Eq. (4), except that b has been replaced by the known derivative $\partial J/\partial x$. The adjoint state λ represents the change in response measure J caused by a unit change in the value of b. The response measure sensitivity in Eq. (6) becomes:

$$\frac{dJ}{du} = \frac{\partial J}{\partial u} + \lambda\left(\frac{\partial b}{\partial u} - \frac{\partial a}{\partial u}x\right) \tag{9}$$

where x is the solution of the state equation, λ is the solution of the adjoint equation, and all derivatives shown are easily found. Thus, with the adjoint method only two simulation runs are required, one each for the state and adjoint equations, in order to determine sensitivity derivatives for <u>all</u> parameters of interest for a given response measure J. In large scale simulations this implies significant cost savings for the calculation of sensitivities.

Suppose that in our simple example J = x, then from Eq. (8) $\lambda = 1/a$ and from Eq. (9):

$$\frac{dJ}{da} = 0 + \frac{1}{a}(0-x) = \frac{-b}{a^2} \quad (10a)$$

$$\frac{dJ}{db} = 0 + \frac{1}{a}(1-0) = \frac{1}{a} \quad (10b)$$

which are the derivatives we earlier calculated by direct differentiation.

Discussion

This simple example has a direct analogy to thermomechanical models. The parameters a and b in our simple state equation, Eq. (4), are analogous to the stiffness matrix and load vector, respectively. This analogy explains why we've written a^{-1} rather than 1/a in Eqs. (6) and (7). The relationship J[u,x(u)] is analogous to the ancilliary calculations that are performed to find, for example, a stress or strain. We'll use this analogy below to write down the adjoint method for a linear thermomechanical model.

The derivation presented here is specific to problems which are linear in state. It is presented as an introduction to the adjoint approach. Nonlinear problems, which we commonly encounter in thermomechanical models, can be solved using a generalization of this derivation. For these problems variations or differentials are used, rather than derivatives. Also, a weaker definition of what is differentiable is admissible, and consequently significant nonlinearities can be treated[1,2,5,6].

LINEAR THERMOMECHANICAL MODEL

The state equations for a finite element linear thermomechanical model are:

$$\underline{K}\,\underline{d} = \underline{f} \quad (11)$$

where $\underline{K}$ is the system stiffness matrix, $\underline{d}$ is the displacment vector and $\underline{f}$ is the load vector of point loads, surface tractions, body forces, and thermal loads. Note that all vectors are written as column vectors; row vectors are written as transposed column vectors. The adjoint equation can be found by following a derivation analogous to that presented for our simple example. If we treat temperature as a prescribed parameter we find:

$$\underline{K}^T\,\underline{\lambda} = \frac{\partial J}{\partial \underline{d}} \quad (12)$$

where λ is the adjoint state vector, superscript T represents a transpose, and $\underline{K}^T = \underline{K}$. $\partial J/\partial \underline{d}$ is an easily filled adjoint load vector. The sensitivity derivative for a parameter u is given by:

$$\frac{dJ}{du} = \frac{\partial J}{\partial u} + \underline{\lambda}^T\left(\frac{\partial \underline{f}}{\partial u} - \frac{\partial \underline{K}}{\partial u}\,\underline{d}\right) \quad (13)$$

Note that parameter u now represents an element property, a traction, a temperature change, etc. The derivatives in this equation are easily filled. Some examples are given in the Appendix.

The adjoint state vector λ represents the change in the value of the response J caused by a unit load at a finite element node point. There are two values of λ at each node point, one for an x-direction applied load and one for a y-direction applied load. The larger the adjoint state, the more influence that an applied nodal force, and its neighboring and intervening properties, have on the response measure.

The sensitivity derivative for each individual parameter is calculated through Eq. (13), but what about the sensitivity to several parameters changing together? Suppose Young's modulus is assumed to be constant in the modeled domain. The parameter sensitivities examined through Eq. (13) with our finite element code involve element values of Young's modulus, that is $u = E^e$. The sensitivity to the assumed domain value, E, is given by:

$$\frac{dJ}{dE} = \sum_{\substack{\text{all}\\ \text{elements}}} \left(\frac{dJ}{dE^e}\right) \quad (14)$$

If the temperature change ΔT over the domain is uniform we have[b]:

$$\frac{dJ}{d(\Delta T)} = \sum_{\substack{\text{all}\\ \text{elements}}} \left[\frac{dJ}{d(\Delta T)^e}\right] \quad (15)$$

but if the change is non-uniform there is a problem. One solution to this and similar problems is to introduce logarithmic sensitivities:

$$\frac{d(\ell n J)}{d(\ell n u)} = \frac{u}{J}\frac{dJ}{du} \quad (16)$$

This expression represents the percent change of response measure J to a one percent change of parameter u. When the temperature change is non-uniform:

$$\frac{d(\ell n J)}{d(\ell n \Delta T)} = \sum_{\substack{\text{all}\\ \text{elements}}} \frac{d(\ell n J)}{d(\ell n \Delta T^e)} \quad (17)$$

where $d(\ell n\Delta T^1) = d(\ell n\Delta T^2) = \ldots = d(\ell n\Delta T^e)$. Equation (17) represents the percent change of the response function for a one percent change of each temperature in the domain. Logarithmic sensitivities also allow the relative comparison and ranking of the sensitvities to widely different parameter types.

As applied to the linear finite element thermomechanical model, the adjoint methods works as follows:

1. Select response functions J.
2. Estimate parameters u including temperatures.
3. With the given u's solve the state equation, Eq. (11), for displacements d.
4. Perform ancilliary calculations to find stresses, and response functions J.
5. Fill derivatives $\partial f/\partial u$ and $\partial K/\partial u$ in Eq. (13).
6. For each J fill derivatives $\partial J/\partial u$ and $\partial J/\partial \underline{d}$ in Eq. (13) and (12) respectively.
7. For each J solve the adjoint equation, Eq. (12), for the adjoint state λ.
8. For each J calculate dJ/du via Eq. (13) for individual parameters u.
9. For domain values of parameters u solve for dJ/du using equivalent of Eq. (14), or logarithmic version, Eq. (17).

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b Temperatures actually vary within the element; the element notation ΔT^e used here is simply representational.

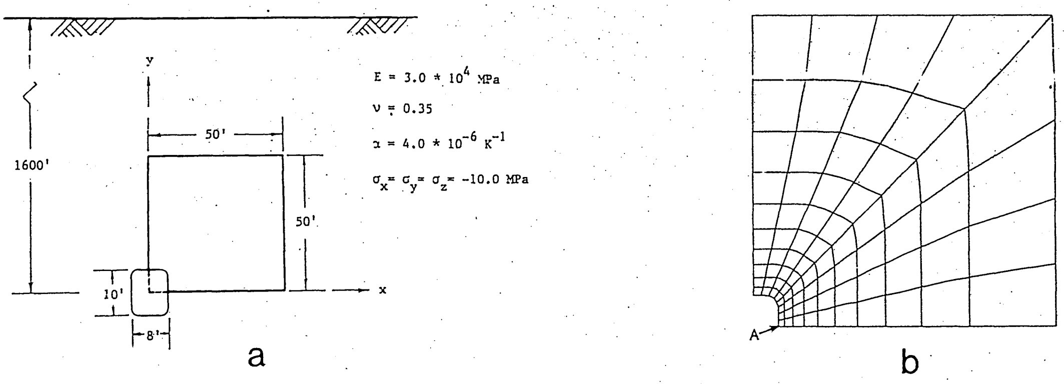

Fig. 2. Application Problem - repository corridor in rock matrix (a) conceptualization (b) finite element mesh.

10. Compare and rank parameters using logarithmic sensitivites.
11. Project response to other parameter assumptions using the multiple parameter version of Eq. (?):

$$J_{new} \simeq J_{old} + \delta J \qquad (18a)$$

$$\delta J \simeq \sum_{\substack{\text{all} \\ \text{parameters}}} \frac{dJ}{du} \delta u$$

$$\simeq J_{old} * \sum_{\substack{\text{all} \\ \text{parameters}}} \frac{d(\ln J)}{d(\ln u)} \delta(\ln u) \qquad (18b)$$

where δ() represents the variation of the quantity in parentheses, such as parameter u; δu. Recall by analogy to the example of Fig. 1 that this projection is only a first order approximation.

Using second-moment probability methods the sensitivites calculated with this method can also be used to obtain first order approximations of uncertainty (the variance) of the predicted response measure.

APPLICATION

Problem

Consider the cross-sectional view of a repository corridor in a rock matrix shown in Fig. 2. A finite element mesh containing 80 isoparametric 8-noded elements was used in a plane strain model of one quarter of the opening. The in situ stresses were assumed constant over the modeled depth and the whole region was subject to a temperature rise ΔT = 25 C. For the parameters given, the displacement and stress fields induced by the opening and temperature rise are plotted in Fig. 3 and Fig. 4, respectively. Take as a response measure the vertical stress, σ_y, at the point marked 'A' in Fig. 2 (the first 2 x 2 Gauss point to the right and above the corner node point). It has a value J = -18.36 MPa.

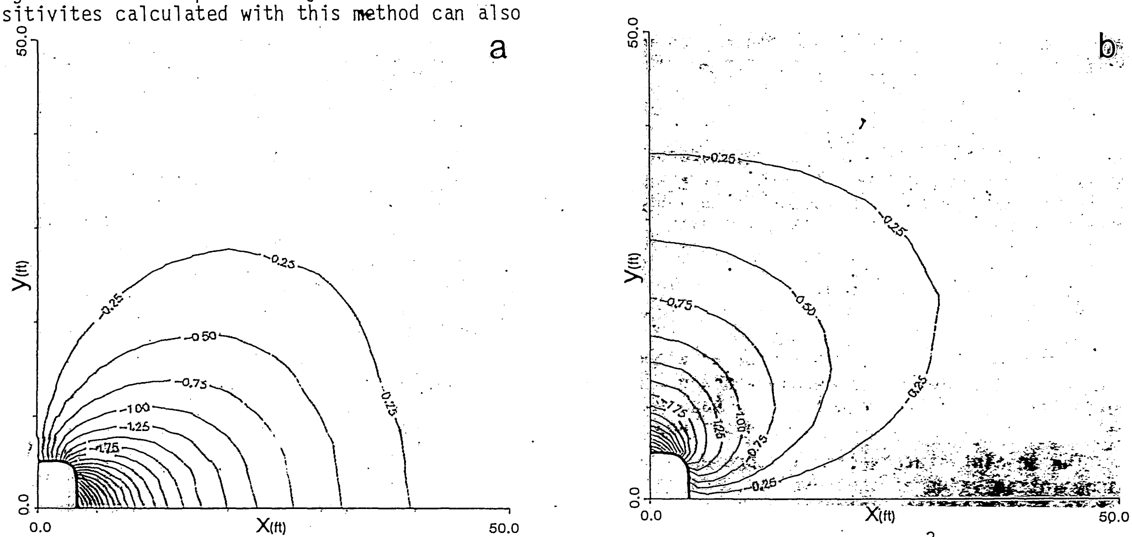

Fig. 3. Contours of displacement around repository corridor (a) x-displacement ($*10^3$)(ft). (b) y-displacement ($*10^3$)(ft).

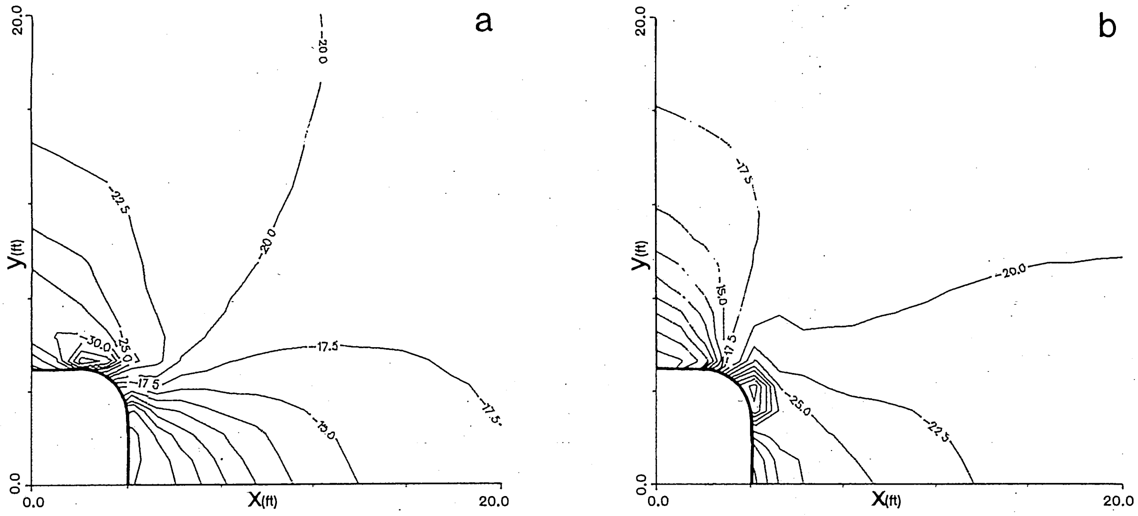

Fig. 4. Contours of stress around repository corridor (a) σ_x (MPa) (b) σ_y (MPa).

Sensitivity Analyses

Figure 5 is a plot of the adjoint state for this response measure and the assumed parameters of the model. There is one adjoint state value for each degree of freedom in the system. For the x-direction the numerically largest value is -1.07; this occurs at A (Fig. 2) and represents the change in the response measure caused by a unit load in the x-direction at that node point. In the y-direction the largest value is 1.49 just above point A. This represents the change in the vertical stress at A caused by a unit nodal load in the y-direction at that point. Adjoint state plots are useful because they quickly identify regions where changes in loading, however induced, will have the greatest effect on the response measure. Intuitively one would expect the adjoint state to become small as the distance from A increases, and indeed this is so.

Sensitivities to element values of Young's modulus E are plotted in Fig. 6. The corresponding numbers are given in Table I. The plot reveals that, away from the opening, there is a definite line dividing positive and negative sensitivities for this parameter. Sensitivities become smaller away from the opening. For E the response measure is most sensitive to the value in the corner element (caused by the first term in Eq. 9). This high sensitivity extends to the adjacent element in row 2, column 2 (Fig. 6 and Table I). Changing Young's modulus in this element causes a greater disturbance in the stress flow (which is normal to the stress contours of Fig. 4) than in other adjacent elements. Note that these sensitivities are unique to the finite element grid used; second-moment probability methods are required to relate element property sensitivities to rock continuum properties. The logarithmic sensitivities of each of the domain parameters, E, Poisson's ratio ν, the

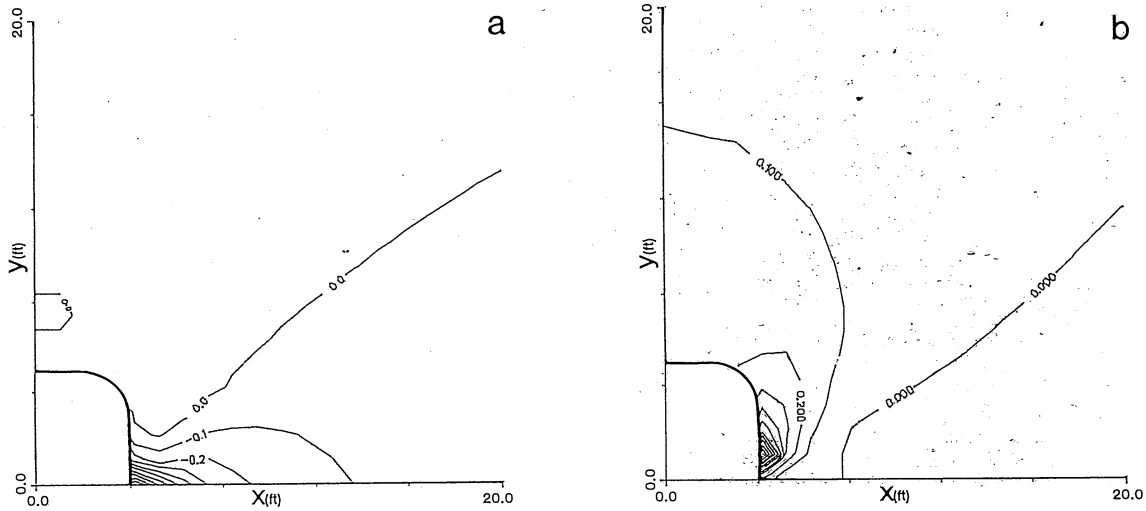

Fig. 5. Contours of adjoint state λ for stress response measure (a) x-direction components (b) y-direction components.

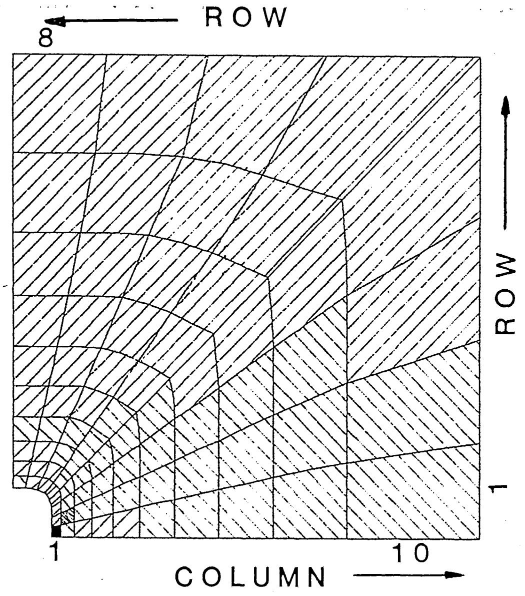

Fig. 6. Sensitivity (Eq. 13) to element values of Young's modulus (shading density ∝ sensitivity; a positive slope indicates a negative sensitivity or an increase in compressive stress J).

coefficient of thermal expansion α and the temperature rise ΔT are given in Table II. The response measure is most sensitive to the domain value of Poisson's ratio and is then equally sensitive to the other domain parameters given in the table. It is to be expected that these sensitivities would be equal because these parameters occur only as a product in the thermal loading term and mechanical stresses are independent of the domain value of Young's modulus in this example.

Using parameter perturbation it would have taken a minimum of five runs to obtain the domain parameter sensitivities of Table II, and 81 runs to obtain the element parameter results of Table I (1 element parameter x 80 elements + base run). The adjoint method required only two runs to obtain all of this information, element parameter sensitivities for ν and α, plus sensitivities to in situ stress that we have not presented.

TABLE I. Sensitivity (Eq. 13) of response measure J to element values of Young's modulus E. (Row and column numbers refer to Fig. 6).

Row	Column 1	2	3	4	5	6	7	8	9	10
8	.20E-5	-.29E-5	-.86E-6	.24E-6	-.16E-5	-.48E-5	-.83E-5	-.12E-4	-.18E-4	-.28E-4
7	-.46E-5	-.59E-5	-.30E-6	.58E-6	-.16E-5	-.45E-5	-.76E-5	-.11E-4	-.16E-4	-.24E-4
6	-.22E-4	-.19E-5	.30E-5	.18E-5	-.85E-6	-.33E-5	-.57E-5	-.87E-5	-.13E-4	-.18E-4
5	-.36E-4	.65E-5	.70E-5	.32E-5	.32E-6	-.17E-5	-.34E-5	-.60E-5	-.11E-4	-.13E-4
4	-.51E-4	.20E-4	.14E-4	.56E-5	.20E-5	.17E-6	-.10E-5	-.26E-5	-.57E-5	-.11E-4
3	-.73E-4	.57E-4	.30E-4	.11E-4	.43E-5	.24E-5	.18E-5	.14E-5	.58E-6	-.28E-5
2	-.76E-4	.13E-3	.35E-4	.56E-5	.22E-5	.32E-5	.41E-5	.48E-5	.54E-5	.66E-5
1	.22E-3	.78E-5	-.43E-4	-.23E-4	-.68E-5	.14E-5	.48E-5	.66E-5	.79E-5	.12E-4

TABLE II. Relative sensitivities of domain parameters.

Domain Parameter u	Logorithmic Sensitivity d(ℓnJ)/d(ℓnu)
E	-0.0448
ν	-0.1693
α	-0.0448
ΔT	-0.0448

DISCUSSION

This simple introduction to the adjoint method has under-emphasized the power of the method for sensitivity analysis, while also down playing its limitations. If we had examined a thermomechanical problem in which temperature was a state, not a parameter, then we would have also had to solve an adjoint problem for the thermal equation. If the system had been nonlinear then we would have given an equivalent nonlinear (actually linearized) adjoint solution. If the response measure had been more complicated, for example, the size of the zone of inelastic behavior in a nonlinear model, the adjoint problem can often be solved. Yet the utility of the adjoint method in application is limited. It provides an exact derivative of the response measure for the assumed parameters of the state equation. Using it to project the response behavior for other parameter values is only first order correct. If some parameter values are highly uncertain, and if the response measure is a significantly nonlinear function of these uncertain parameters, then first order projection of behavior may be inadequate. In this case systematic multiple simulation runs with varying parameters are necessary. The adjoint method is not a panacea, but a tool. One that is used together with other tools to provide a better understanding of thermomechanical behavior and our ability to make confident predictions.

The major utility of the adjoint method is the large amount of sensitivity information that a single additional run of the simulation code provides. The adjoint state is itself an important measure of system behavior, and in some other fields is often the total focus of the adjoint approach. The calculated parameter sensitivities can be used to improve model conceptualizations, to guide laboratory and field testing, and to improve repository design.

The adjoint method can be crudely applied to existing thermomechanical codes with little or no internal revision. The existing code can usually be arranged as a large 'macro' in a new driving routine. However, for nonlinear problems this could easily lead to incorrect adjoint solutions. Reprogramming a complex nonlinear code to solve the adjoint problem and correctly calculate the sensitivity derivatives can be a time consuming and laborious task. The additional information that is yielded by doing this is only justified if the code is to be frequently used.

We've given one demonstration example of the adjoint method. Although these results are application specific, several generalizations can be drawn:

- The adjoint method is a relatively inexpensive and efficient means of obtaining parameter sensitivity derivatives.

- The adjoint state is of value in itself since it can be used to identify regions where a change in applied load will have the most influence on the response function.

- The logorithmic sensitivities provide a means of comparing the influence that different system parameters have on a given response measure. They are not useful in determining how sensitive the response measure is to spatial variations in parameters.

- On the other hand, a sensitivity plot such as the one in Fig. 6 can show the relative importance of a particular element parameter. Such a map can provide not only the sign and relative magnitude of the sensitivity to a given element parameter, but can also identify critical regions in the domain.

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APPENDIX

The derivatives $\partial J/\partial d$, $\partial J/\partial u$, $\partial f/\partial u$ and $\partial K/\partial u$ are easily filled on an element basis. For the sake of explanation, however, global matrix notation is used for these examples.

Let's take the x-direction stress at a prescribed point x_0 as the response measure of interest. Then $J = \sigma_x$ is the x-direction component of the local stress vector:

$$\underset{\sim}{\sigma} = \underset{\sim}{\sigma}^0 + \underline{D}\,\underline{B}\,\underline{d} - \underline{D}\,\underset{\sim}{\varepsilon}^0 \tag{19}$$

where $\underline{D}$ is the compliance elasticity matrix, $\underline{B}$ is the strain matrix, $\underset{\sim}{\sigma}^0$ is the initial stress, and $\underset{\sim}{\varepsilon}^0$ is the initial thermal strain. We find:

$$\frac{\partial J}{\partial u} = \frac{\partial J}{\partial \underset{\sim}{\sigma}^T}\left(\frac{\partial \underset{\sim}{\sigma}^0}{\partial u} + \frac{\partial \underline{D}}{\partial u}(\underline{B}\,\underline{d} - \underset{\sim}{\varepsilon}^0) - \underline{D}\frac{\partial \underset{\sim}{\varepsilon}^0}{\partial u}\right) \tag{20}$$

$$\frac{\partial J}{\partial \underline{d}^T} = \frac{\partial J}{\partial \underset{\sim}{\sigma}^T}\underline{D}\,\underline{B} \tag{21}$$

Since $J = \sigma_x$, then $\partial J/\partial \underset{\sim}{\sigma}^T = \{1,0,0,0\}$ for two-dimensional or axisymmetric problems. Equation (21) is used to fill the adjoint load vector in Eq. (12), while Eq. (20) represents the direct sensitivity of J to u.

The derivatives of the stiffness matrix and load vector are needed to complete Eq. (13). Suppose we're interested in Young's modulus E in element e. It affects the stiffness matrix $\underline{K}$ and the thermal load contribution, $\underline{f}^t$, to vector $\underline{f}$. Both $\underline{K}$ and $\underline{f}^t$ are linear in E^e, so that these derivatives are simply given by:

$$\frac{\partial \underline{K}}{\partial u} = \frac{\partial \underline{K}}{\partial E^e} = \underline{K}^* \tag{22}$$

$$\frac{\partial \underline{f}}{\partial u} = \frac{\partial \underline{f}}{\partial E^e} = \frac{\partial \underline{f}^t}{\partial E^e} = \underline{f}^{t*} \tag{23}$$

in which all the element values of E in $\underline{K}$ or $\underline{f}^t$ are replaced by zero's, except for element e, in which it is replaced by unity. Also Eq. (20) becomes:

$$\frac{dJ}{du} = \frac{\partial J}{\partial \underset{\sim}{\sigma}^T}\underline{D}^*(\underline{B}\,\underline{d} - \underset{\sim}{\varepsilon}^0) \tag{24}$$

in which the same thing occurs to $\underline{D}$.

The examples given in Eqs. (19) to (24) are simply illustrative. We've developed and coded stiffness matrix and load vector derivatives for all of the parameters occuring in the models we've been examining, as well as partial derivative Eqs. (20) and (21) for a wide variety of response measures.