DEVELOPMENT AND IMPLEMENTATION OF SENSITIVITY COEFFICIENT EQUATIONS FOR HEAT CONDUCTION PROBLEMS

Ben F. Blackwell, Robert J. Cochran, and Kevin J. Dowding
Engineering Sciences Center
Sandia National Laboratories
Albuquerque, NM 87185-0835

Abstract

Three different methods are discussed for computing the sensitivity of the temperature field to changes in material properties and initial/boundary condition parameters for heat conduction problems. The most general method is to derive sensitivity equations by differentiating the energy equation with respect to the parameter of interest and numerically solving the resulting sensitivity equations. An example problem in which there are twelve parameters of interest is presented and the resulting sensitivity equations are derived. Numerical results are presented for thermal conductivity and volumetric heat capacity sensitivity coefficients for heat conduction in a 2-D orthotropic body. The numerical results are compared with the analytical solution to demonstrate that the numerical method is second order accurate as the mesh is refined spatially.

Nomenclature

A area, m²
C = ρcₚ volumetric heat capacity, J/m³-°C
cₚ heat capacity, J/kg-°C
e'' energy source, W/m³
h convective heat transfer coefficient, W/m²-°C
k thermal conductivity, W/m-°C
kᵢᵢ principal component of thermal conductivity tensor, W/m-°C

1. This work was performed at Sandia National Laboratories and supported by the U. S. Department of Energy under Contract DE-AC/04-94AL85000.
DRAFT

\( \tilde{k} \) thermal conductivity tensor
\( L \) thickness of slab, m
\( N_p \) number of sensitivity coefficients
\( \hat{n} \) unit normal vector
\( \hat{p} \) parameter vector
\( p_i \) element of \( \hat{p} \)
\( q'' \) heat flux, W/m\(^2\)
\( q''_c \) convective heat flux, W/m\(^2\)
\( q''_o \) constant value of heat flux, W/m\(^2\)
\( q''_r \) radiative heat flux, W/m\(^2\)
\( T \) temperature, °C
\( T_b \) boundary temperature, °C
\( T_o \) initial temperature, °C
\( T_{p_i} \) temperature sensitivity coefficient for parameter \( p_i \), °C
\( T_r \) radiation temperature, °C
\( T_{\infty} \) convection temperature, °C
\( V \) volume, m\(^3\)
\( X \) dimensionless sensitivity coefficient
\( X_{k_a} \) analytically determined value of dimensionless thermal conductivity sensitivity coefficient
\( X_{k_n} \) numerically determined value of dimensionless thermal conductivity sensitivity coefficient
\( x \) spatial coordinate, m
\( \hat{x}_b \) position vector along boundary, m

Greek
\( \alpha = k/\rho c_p \), thermal diffusivity, m\(^2\)/s
\( \varepsilon \) emittance
\( \rho \) density, kg/m\(^3\)
\( \sigma \) Stefan-Boltzmann constant
\( \phi \) dimensionless temperature rise
DISCLAIMER

This report was prepared as an account of work sponsored by an agency of the United States Government. Neither the United States Government nor any agency thereof, nor any of their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency thereof. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or any agency thereof.
1.0 Introduction

In the process of performing thermal analysis/design studies, most analysts/designers have asked themselves the question “what happens to the temperature field if the thermal conductivity of one of the materials decreases” or “what happens to the maximum temperature if the heat flux is increased?” This leads to additional simulations in which you vary the model parameter(s) of interest. In essence, the analyst is computing what are termed “sensitivity coefficients.” Within the context of this paper, sensitivity coefficients are defined as partial derivatives of field variables (temperature, displacement, velocity, etc.) with respect to model parameters (conductivity, Young’s modulus, viscosity, etc.). Sensitivity coefficients are useful for a wide variety of problems, including estimation of material properties, boundary conditions, source terms, etc., from field measurements, optimal design of experiments, uncertainty analysis, optimization, and design/analysis studies.

The structural analysis community is far ahead of the heat transfer community in the utilization of sensitivity coefficients. An introduction into the structural analysis literature can be found in Kleiber and Hien (1992) and Kleiber, et al. (1997). In the thermal parameter estimation arena (including the inverse heat conduction problem), a representative sample of references using sensitivity coefficients can be found in Beck and Arnold (1977); Beck et al. (1985); Blackwell and Eldred (1997); Dowding, et al. (1995); Dowding, et al. (1996); Fadale, et al. (1995); Osman, et al. (1997); and Tseng and Zhao (1996). In the optimum design of thermal experiments, a representative sample of references using sensitivity coefficients can be found in Beck and Arnold (1977); Emery and Fadale (1996a); Emery and Fadale (1997); and Emery, et al. (1997). In the thermal uncertainty analysis area, a representative sample of references using sensitivity coefficients can be found in Emery and Fadale (1996b), Fadale (1993), and Fadale and Emery (1994). In the thermal optimization area, a representative sample of references using sensitivity coefficients can be found in Hafkka (1981) and Tortorelli and Michaleris (1994).

In the course of performing a parameter study of a particular design, analysts look at sensitivity coefficients. In many cases, the term “sensitivity coefficient” may not even be used. Instead, statements like “if the thermal conductivity decreased, the surface temperature where the heat flux was applied will increase” are made. The implication of this statement is that the sensitivity coefficient \( \frac{\partial T}{\partial k} \) is negative. In a preliminary design study, the sign of the sensitivity coefficient may be all that is required. However, if the magnitude of the sensitivity coefficient is known, then much more information is available. This is demonstrated by looking at a simple example of a Taylor series expansion of the temperature field in terms of a single parameter, such as the thermal conductivity;

\[
T(k) = T(k^0) + \left. \frac{\partial T}{\partial k} \right|_{k^0} (k - k^0) + \ldots \tag{1.1}
\]

where \( k^0 \) is the “nominal” value of thermal conductivity. If \( T(k^0) \) and \( \left. \frac{\partial T}{\partial k} \right|_{k^0} \) are known, then the temperature field at the perturbed value of conductivity \( k \) can be approximated from Eq. (1.1), provided that the perturbation in thermal conductivity is sufficiently small that a first order
Taylor series expansion is valid. In preliminary design studies, the linear (or first order) assumption is often adequate.

Sensitivity coefficients are generally determined by one of three methods: 1) analytical differentiation of analytical solutions for the temperature field (termed "analytical"); 2) numerical differentiation of numerical solutions for the temperature field (termed "finite difference"), and 3) direct differentiation of governing equations and numerical solution of the resulting equations (termed "direct differentiation"). In the following sections, we will discuss each of these three methods.

2.0 Analytical Determination of Sensitivity Coefficients

If the temperature field is known analytically, the solution can be analytically differentiated with respect to the parameters of interest to obtain sensitivity coefficients. In order to solidify some of the sensitivity coefficient concepts, let us consider an example for which an analytical solution exists for the temperature field. This allows analytical determination of the sensitivity coefficients. Figure 2-1 is a schematic of a 1-D transient heat conduction problem for which an analytical solution can be used to obtain sensitivity coefficients; this problem is also discussed in Beck and Arnold (1977). From Beck and Arnold (1977, p. 454) or Beck, Blackwell, and St. Clair (1985, p. 14) the analytical solution to this problem is given by

\[
\phi = \frac{T - T_o}{q''L} = \frac{\alpha t}{L^2} + \frac{1}{3} - \frac{x}{L} + \frac{1}{2} \left( \frac{x}{L} \right)^2 - \frac{2}{\pi^2} \sum_{n=1}^{\infty} \frac{1}{n^2} \exp \left( -n^2 \pi^2 \frac{\alpha t}{L^2} \right) \cos \pi \frac{x}{L} 
\]

(2.1)

where the thermal diffusivity is the ratio of thermal conductivity to volumetric heat capacity (\(\alpha = k/C\)). We want to compute the sensitivity of the temperature field to the heat flux, thermal conductivity, and volumetric heat capacity. Solving for temperature in Eq. (2.1) gives

\[
T = T_o + \frac{q''L}{k} \phi \left( \alpha, \frac{x}{L}, \frac{t}{L^2} \right). 
\]

(2.2)

Differentiating Eq. (2.2) with respect to the heat flux,
This sensitivity coefficient has units of \([T]/[q''']\); other sensitivity coefficients will have totally different units. In order to compare the effects of changing various parameters, it will be convenient to scale each sensitivity coefficient such that they have units of temperature. This can be done by multiplying each sensitivity coefficient by its respective parameter\(^1\). For the heat flux sensitivity coefficient, this becomes\(^2\)

\[
T_{q'} = q''' \frac{\partial T}{\partial q'''} = \frac{\partial T}{\partial \ln q'''} = \frac{q'''}{k} \frac{\partial T}{\partial \ln q'''} = \frac{q'''}{k} \frac{\partial T}{\partial \ln q'''} = \phi.
\]

The coefficient of \(\phi\) in Eq. (2.4) has the units of temperature and if we use that as a normalizing factor, a dimensionless sensitivity coefficient can be defined as

\[
X_{q'} = \frac{T_{q'}}{q'''} = \phi.
\]

The dimensionless heat flux sensitivity coefficient is simply the dimensionless temperature response.

Next we compute the sensitivity with respect to the volumetric heat capacity \(C\). Differentiating Eq. (2.2) and using the chain rule,

\[
\frac{\partial T}{\partial C} = \frac{q'''}{k} \frac{\alpha \partial \phi}{C \partial \alpha}.
\]

The scaled and dimensionless volumetric heat capacity sensitivity coefficients are

\[
T_C = C \frac{\partial T}{\partial C} = \frac{q'''}{k} \frac{\alpha \partial \phi}{C \partial \alpha}, \quad X_C = \frac{C \frac{\partial T}{\partial C}}{q'''} = -\frac{\alpha \partial \phi}{q''' \partial \alpha}.
\]

For the thermal conductivity,

---

1. This process is equivalent to taking the derivative of the field variable with respect to the logarithm of the parameter and will be referred to as the logarithmic derivative.

2. The subscript notation for scaled sensitivity coefficients is designed to emphasize that the units are temperature and to identify the variable for which we are computing the sensitivity. Unfortunately, this notation is in conflict with the common mathematical notation that a subscript denotes partial differentiation only, and not the scaled version. The notation presented here will be useful for multimechanics problems in which sensitivity coefficients are considered for many different field variables.
By differentiating Eq. (2.1) with respect to thermal diffusivity, we obtain

\[ T_k = k \frac{\partial T}{\partial k} = \frac{q'' L}{k} \left( \alpha \frac{\partial \phi}{\partial \alpha} - \phi \right), \quad X_k = \frac{k}{q'' L} \frac{\partial T}{\partial k} = \alpha \frac{\partial \phi}{\partial \alpha} - \phi. \tag{2.8} \]

All the pieces are available to compute the three sensitivity coefficients. The dimensionless heat flux sensitivity coefficient is shown in Figure 2-2. The heat flux sensitivity coefficient is always positive; increasing the heat flux increases the temperature for all times and depths. The closer one goes to the heated surface, the greater is the sensitivity coefficient. For a fixed value of time, the sensitivity coefficient is a nonlinear function of position. As time increases, the sensitivity coefficients increase without bound; this implies that an increase in heat flux has a greater impact on the temperature at late time than at early time. This is a consequence of this problem not having a steady state solution. For large values of time, the sensitivity coefficient approaches a linear function of time. Most of these conclusions are obvious for an experienced thermal analyst, so one might ask why bother? First, an inexperienced thermal analyst has to develop intuition and

FIGURE 2-2: Dimensionless heat flux sensitivity coefficient as a function of dimensionless time for various depths below the heated surface.
sensitivity coefficients can aid this learning process. Second, when the geometry and/or boundary conditions are sufficiently complicated that one's intuition cannot be relied upon (in some cases intuition actually misleads us), then one must look at something like sensitivity coefficients.

The volumetric heat capacity sensitivity coefficients are shown in Figure 2-3. They are negative for all values of time and position; an increase in volumetric heat capacity causes a decrease in temperature. The sensitivity coefficient has the largest magnitude for locations near the heated surface. For large values of time, the sensitivity coefficients become independent of position and approach a linear relationship with time. For locations near the heated surface, the temperature is more sensitive to changes in heat flux than to changes in volumetric heat capacity. However, for locations near the adiabatic surface, the temperature is more sensitive to changes in volumetric heat capacity than to heat flux; this conclusion would be difficult to ascertain solely by intuition and, hence, demonstrates the power of sensitivity coefficients. Recall that because the sensitivity coefficients are scaled, their magnitudes can be directly compared.

The thermal conductivity sensitivity coefficient is shown in Figure 2-4. This sensitivity coefficient is quite different from the heat flux and volumetric heat capacity sensitivity coefficients because it can be either positive or negative, depending on depth below the heated surface and time. Near the heated surface, the sensitivity coefficient is negative, indicating that an increase in thermal conductivity causes a decrease in temperature. At the adiabatic surface the sensitivity coefficient is positive, indicating an increase in thermal conductivity causes an increase in temperature. Consequently, for a given value of time, there is a position for which the sensitivity coefficient is zero. This indicates a position of insensitivity to changes in thermal conductivity. The spatial location
where the sensitivity coefficient is zero changes with time. For $x/L = 0.25$, the sensitivity coefficient is positive initially but becomes negative at later times. If one were taking experimental measurements of temperature in order to estimate thermal conductivity, then sensors in the range $0.3 < x/L < 0.5$ would provide very little information. In some circumstances, it might be desirable to place temperature sensors in locations where the indicated temperature is insensitive to the local thermal conductivity. Quantitative information of this kind is difficult to obtain without the aid of sensitivity coefficients. The results in Figure 2-4 suggest that for long times ($\alpha t/L^2 > 0.5$), the sensitivity coefficient approaches an asymptotic value independent of time. This can be confirmed by looking at the long time limit of $X_k$:

$$X_k|_{t \to \infty} = -\left[\frac{1}{3} \frac{x}{L} + \frac{1}{2} \left(\frac{x}{L}\right)^2\right].$$

For large times, the heat flux and volumetric heat capacity sensitivity coefficients dominate the thermal conductivity sensitivity coefficient. From the analytical results presented, one can demonstrate that the three dimensionless sensitivity coefficients discussed sum to zero for all values of time and position.

$$X_{q''} + X_C + X_k = 0.$$ 

This result says that the three sensitivity coefficients are not independent. It is not possible to simultaneously estimate $(q'', C, k)$ from temperature measurements in this configuration. This

**FIGURE 2-4**: Dimensionless thermal conductivity sensitivity coefficient as a function of dimensionless time for various depths below the heated surface.
could have been anticipated by observing that in Eq. (2.1), the temperature depends only on the ratio of $\dot{q}''/k$ and $k/C$; consequently, these three sensitivity coefficients are not independent. In more complicated situations for which analytical solutions are not available, it may be difficult to ascertain independence of the sensitivity coefficients. Beck and Arnold (1977) and Marchall and Milos (1997) discuss techniques for judging the independence of sensitivity coefficients.

Additional discussion of sensitivity coefficients for this problem can be found in Beck and Arnold (1977, pp. 454-457).

### 3.0 Finite Difference Determination of Sensitivity Coefficients

In general, one resorts to numerical solutions for many real world problems. For this case, sensitivity coefficients are often computed using a first order backwards difference of the form:

$$\frac{\partial T}{\partial k} \bigg|_{k^o} = \frac{T(k^o + \Delta k) - T(k^o)}{\Delta k} + O(\Delta k), \quad k \frac{\partial T}{\partial k} \bigg|_{k^o} = \frac{k^o T(k^o + \Delta k) - T(k^o)}{\Delta k}. \quad (3.1)$$

For the case of a single sensitivity coefficient, two solutions for the temperature field are required; one for $T(k^o + \Delta k)$ and one for $T(k^o)$. For $n$ parameters and a first order accurate backwards difference, the scaled sensitivity coefficients can be computed from

$$T_{p_i} = \frac{p_i T(p_1, p_2, \ldots, p_i + \Delta p_i, \ldots, p_n) - T(p_1, p_2, \ldots, p_i, \ldots, p_n)}{\Delta p_i}. \quad (3.2)$$

This approach will require $n+1$ solutions for the temperature field. If a second order accurate central difference is used, then $2n+1$ solutions of the temperature field will be required. There are many examples in the literature where this approach has been successfully used. An advantage of this approach is that (for this example) you numerically solve the problem with different inputs. No source code modification is required; this can be a significant cost advantage for this method.

Some numerical experimentation is strongly recommended to determine an acceptable value for the finite difference step size. If it is too large, the truncation errors will be excessive; if it is too small, machine round off may become a problem. In order to emphasize the importance of this issue, consider the example problem given in Figure 2-1. This example was solved numerically using a control volume finite element code with a lumped capacitance matrix and a fully implicit time integrator; double precision on a 32-bit machine (nominally 15 digits) was utilized. The final problem time was 20 s, which corresponded to a dimensionless time ($at/L^2$) of 0.5. The sensitivity coefficient with respect to thermal conductivity was computed for the node at $x=0$ for $t=20$ s.

---

1. The use of the term “finite difference” in this context should not be confused with the finite difference method of discretizing partial differential equations. The methodology discussed here for computing sensitivity coefficients can be utilized with any discretization method (finite difference, Galerkin finite element, control volume finite element, etc.) for partial differential equations.
utilizing a range of values for $\Delta k$ for a backwards difference approximation. The relative error in each computation was computed from

\[
\text{\% Error} = 100 \frac{X_{kn} - X_{ka}}{X_{ka}}
\]  

(3.3)

where the subscripts $n$ and $a$ represent numerical and analytical respectively; the error results are presented in Figure 3-1. Uniform grids of 10 and 20 elements were used along with a fixed time step of $\Delta t = 0.1$ s. Focusing on the upper right hand corner of this figure and the double precision (DP) results, as you decrease the relative finite difference step size ($\Delta k/k$), the error decreases initially and then reaches a plateau. From theoretical considerations of the Taylor series truncation error, the errors in the finite difference sensitivity coefficient (backwards difference) would decay linearly with decreasing finite difference step size. However, there are errors in the predicted temperature field. The curve in Figure 3-1 labeled "first order" is such a linear relationship and is shown for reference. Due to the errors in the numerical solution for the temperature field, it is obvious that the sensitivity coefficient errors do not decay linearly as the finite difference step size is decreased. As the mesh is refined from 10 to 20 elements, the errors are closer to the linear relationship in the upper right hand portion of the figure. Although not shown in Figure 3-1, calculations were performed for relative finite difference step sizes of $10^{-6}$, and they continue the observed plateau. The plateau region double precision results are consistent with those results obtained by the direct differentiation method to be discussed in a subsequent section.

FIGURE 3-1: Sensitivity coefficient errors as a function of $\Delta k/k$ for two different grid refinements (DP is double precision and SP is single precision).
The single precision results in Figure 3-1 were obtained by taking the double precision temperature predictions, truncating them to seven significant digits, and then using finite differences to compute the sensitivity coefficients. There are clearly round off errors for a relative step size below $10^{-5}$. The single precision results in Figure 3-1 have smaller errors than the corresponding double precision results; this is purely coincidental.

In conclusion, grid convergence errors must first be eliminated before one can expect first order accuracy of the finite difference derived sensitivity coefficients. From a practical perspective, a relative finite difference step size of approximately $10^{-4}$ is recommended, provided no other information is available. However, a more reliable method is to perform parameter studies for your particular problem. Calculations are best performed in double precision on 32-bit machines.

4.0 Direct Differentiation (Integral Equation Perspective)

In practical problems, the sensitivity with respect to many different variables is needed. For example, consider the problem shown in Figure 4-1. The four boundary conditions shown here were

\[ -(\tilde{k} \cdot \nabla T) \cdot \hat{n}|_{x_3} = \varepsilon \sigma [T^4(x_3) - T^4_\infty] \]

\[ \frac{\partial T}{\partial t} - \nabla \cdot (\tilde{k} \cdot \nabla T) = \varepsilon'''' \]

\[ -(\tilde{k} \cdot \nabla T) \cdot \hat{n}|_{x_2} = h[T(x_2) - T_\infty] \]

\[ T(x_4) = T_b \]

\[ T(x, 0) = T_o \]

\[ -(\tilde{k} \cdot \nabla T) \cdot \hat{n}|_{x_1} = \dot{q}_o'' \]

chosen because they commonly occur in practice. If we assume that all the material properties, source term, and boundary condition parameters are independent of time/space/temperature and the thermal conductivity tensor is for an orthotropic material, then this problem contains twelve parameters. We will write those parameters as a vector of the form

\[ \hat{p} = \begin{Bmatrix} k_{11} & k_{22} & k_{33} & C \varepsilon'''' & \dot{q}_o'' & h & \varepsilon & T_\infty & T_r & T_b & T_o \end{Bmatrix}^T \]

(4.1)
If Eq. (1.1) is generalized for an arbitrary number of parameters \( n \) and extended to second order accuracy, then

\[
T(\hat{p}) = T(\hat{p}^o) + (\hat{p} - \hat{p}^o) \left[ \frac{\partial T}{\partial \hat{p}} \right] \hat{p}^o + \frac{1}{2} (\hat{p} - \hat{p}^o) \left[ \frac{\partial^2 T}{\partial \hat{p} \partial \hat{p}} \right] \hat{p}^o + \ldots \tag{4.2}
\]

where

\[
\left\{ \frac{\partial T}{\partial \hat{p}} \right\} = \left[ \frac{\partial T}{\partial p_1} \frac{\partial T}{\partial p_2} \ldots \frac{\partial T}{\partial p_n} \right], \quad \left[ \frac{\partial^2 T}{\partial \hat{p} \partial \hat{p}} \right] = \left[ \frac{\partial^2 T}{\partial p_1 \partial p_1} \frac{\partial^2 T}{\partial p_1 \partial p_2} \ldots \frac{\partial^2 T}{\partial p_1 \partial p_n} \right] \ldots \left[ \frac{\partial^2 T}{\partial p_n \partial p_1} \frac{\partial^2 T}{\partial p_n \partial p_2} \ldots \frac{\partial^2 T}{\partial p_n \partial p_n} \right] \tag{4.3}
\]

The notation on the left hand side of the second order sensitivity coefficient matrix is meant to be suggestive and not literal. There are \( n \) first order sensitivity coefficients and \( n^2 \) second order sensitivity coefficients in Eq. (4.3); however, because of the symmetry of the second order sensitivity coefficient matrix, there are only \( n(n + 1)/2 \) distinct second order sensitivity coefficients. For a first order analysis, the computational load will scale linearly with the number of parameters; for a second order analysis, the computational load will scale as the square of the number of parameters. From the computational load perspective, there is strong incentive to perform a first order analysis.

Eq. (4.2) can be written in summation notation as

\[
T(\hat{p}) = T(\hat{p}^o) + \sum_{i=1}^{n} (p_i - p_i^o) \frac{\partial T}{\partial p_i} \bigg|_{\hat{p}^o} + \frac{1}{2} \sum_{i=1}^{n} \sum_{j=1}^{n} (p_i - p_i^o)(p_j - p_j^o) \frac{\partial^2 T}{\partial p_i \partial p_j} \bigg|_{\hat{p}^o} + \ldots \tag{4.4}
\]

The units of the first order sensitivity coefficient are \([T]/[p_i]\). Consequently, it may be difficult to compare the sensitivity coefficients for two different parameters because of the different units. A way around this is to scale each of the sensitivity coefficients by their nominal parameter value.

\[
T_{p_i} = p_i^o \frac{\partial T}{\partial p_i}, \quad T_{p_i p_j} = p_i^o p_j^o \frac{\partial^2 T}{\partial p_i \partial p_j} \tag{4.5}
\]

Now, the scaled sensitivity coefficients all have units of the field variable (temperature in this example) and can be more readily compared. If the scaled sensitivity coefficients are introduced into the Taylor series expansion given by Eq. (4.4), we obtain
\[ T(\beta) = T(\beta^0) + \sum_{i=1}^{n} \delta p_i T_{\beta_i}^\beta + \frac{1}{2} \sum_{i=1}^{n} \sum_{j=1}^{n} \delta p_i T_{p_i,p_j}^\beta \delta p_j + \ldots \]  

(4.6)

where a relative parameter change has been defined as

\[ \delta p_i = \frac{p_i - p_i^0}{p_i^0} . \]  

(4.7)

In the work that follows, we will assume a first order Taylor series is valid and will focus on techniques to compute first order sensitivity coefficients. The same methodology can be extended to higher order sensitivity coefficients if it is deemed necessary.

The details of the Direct Differentiation Method used to calculate sensitivity coefficients is now presented. This method involves taking the governing integral equation along with boundary/initial conditions and differentiating them with respect to the parameter of interest. This process produces integral equations in which the dependent variable is the sensitivity coefficient. The derived sensitivity coefficient integral equations can then be solved by whatever discretization method you choose. Our discretization method is the control volume finite element method; hence our results will be written in terms of integral equations. This process will now be demonstrated by considering the example problem given in Figure 4-1.

The integral form of the energy equation for a heat conducting body is:

\[ \frac{\partial}{\partial t} \int \int \int \nabla \cdot \dot{q} \, d\psi + \int \int \int \ddot{q} \cdot d\mathcal{A} = \int \int \int \dot{e} \, d\psi \]  

(4.8)

where the heat flux vector is given by Fourier's Law,

\[ \dot{q} = -\bar{k} \cdot \nabla T . \]  

(4.9)

and the (orthotropic) thermal conductivity tensor is given by

\[ \bar{k} = \begin{bmatrix} k_{11} & 0 & 0 \\ 0 & k_{22} & 0 \\ 0 & 0 & k_{33} \end{bmatrix} . \]  

(4.10)

The initial/boundary conditions for the problem defined in Figure 4-1 can be written as

\[ T(\dot{\mathbf{x}}, 0) = T_0 . \]  

(4.11)

---

1. The volumetric heat capacity is used in the governing equation because you can not distinguish changes in density from changes in heat capacity.
The three flux type boundary conditions can all be combined into a single equation of the form:

\[- \int \int (\vec{k} \cdot \nabla T)_{b_1} \cdot d\vec{A} = \int \int q_c'' d\vec{A} \]  

\[- \int \int (\vec{k} \cdot \nabla T)_{b_2} \cdot d\vec{A} = \int \int h(T - T_{\infty})_{b_2} \cdot d\vec{A} = \int \int q_c'' d\vec{A} \]  

\[- \int \int (\vec{k} \cdot \nabla T)_{b_3} \cdot d\vec{A} = \int \int \varepsilon \sigma [T^4 - T^4_r]_{b_3} \cdot d\vec{A} = \int \int q_r'' d\vec{A} \]  

\[T(\hat{x}_4) = T_b. \]  

The three flux type boundary conditions can all be combined into a single equation of the form:

\[\int \int \hat{q} \cdot d\vec{A} = \int \int - (\vec{k} \cdot \nabla T)_{b} \cdot d\vec{A} = \int \int \hat{q}'' \hat{n} \cdot d\vec{A} \]  

where

\[\hat{q}'' = \begin{cases} \hat{q}_o'' \text{ along } \hat{x}_{b_1} \\ \hat{q}_c'' = h(T - T_{\infty}) \text{ along } \hat{x}_{b_2} \\ \hat{q}_r'' = \varepsilon \sigma (T^4 - T^4_r) \text{ along } \hat{x}_{b_3} \end{cases}. \]  

If Fourier’s Law is substituted into the energy equation, we obtain

\[\frac{\partial}{\partial t} \int \int_{\Omega} C d\nu + \int \int_{\Omega} \vec{k} \cdot \nabla T \cdot d\vec{A} = \int \int_{\Omega} \varepsilon \sigma (T^4 - T^4_r) \cdot d\vec{A}. \]  

The first step in the sensitivity coefficient determination process is to differentiate the energy equation with respect to an arbitrary element of the parameter vector given by Eq. (4.1) and multiply the result by the parameter vector. Note that the parameter is assumed to be independent of time/space so that it can be moved inside the integral sign. Interchanging the order of differentiation and integration results in:

\[\frac{\partial}{\partial t} \int \int_{\Omega} p \frac{\partial}{\partial p_i} (CT) d\nu + \int \int_{\Omega} p \frac{\partial}{\partial p_i} \hat{q} \cdot d\vec{A} = \int \int_{\Omega} p \frac{\partial}{\partial p_i} \varepsilon \sigma (T^4 - T^4_r) d\nu. \]  

The integrand of the capacitance related term can be written as:

\[p \frac{\partial}{\partial p_i} (CT) = p_i \left( \frac{\partial C}{\partial p_i} T + \frac{\partial T}{\partial p_i} C \right) = C T_{p_i} + p_i \frac{\partial C}{\partial p_i} T. \]  

The single capacitance term in the energy equation becomes two terms in the sensitivity equation; the first term involves the unknown sensitivity coefficient and the second involves the (known)
temperature. Note however, that the only time the second term is non-zero is when \( p_i = C \); i.e., when we are computing the sensitivity with respect to the volumetric heat capacity. This assumes that the parameters are independent of each other.

Fourier’s Law can be written as

\[
\hat{q} = \begin{bmatrix} k_{11} & 0 & 0 \\ 0 & k_{22} & 0 \\ 0 & 0 & k_{33} \end{bmatrix} \begin{bmatrix} \frac{\partial T}{\partial x_1} \\ \frac{\partial T}{\partial x_2} \\ \frac{\partial T}{\partial x_3} \end{bmatrix}.
\]  

(4.21)

Taking the logarithmic derivative of Eq. (4.21) with respect to an arbitrary parameter,

\[
p_i \frac{\partial}{\partial p_i} \hat{q} = -\tilde{k} \cdot \nabla T_{p_i} - p_i \begin{bmatrix} \frac{\partial k_{11}}{\partial p_i} & 0 & 0 \\ 0 & \frac{\partial k_{22}}{\partial p_i} & 0 \\ 0 & 0 & \frac{\partial k_{33}}{\partial p_i} \end{bmatrix} \begin{bmatrix} \frac{\partial T}{\partial x_1} \\ \frac{\partial T}{\partial x_2} \\ \frac{\partial T}{\partial x_3} \end{bmatrix}.
\]  

(4.22)

The only terms in the derivative of the thermal conductivity tensor that are non-zero occur when the parameter \( p_i \) is one of the elements of the thermal conductivity tensor. Consequently, Eq. (4.22) can be written as

\[
p_i \frac{\partial}{\partial p_i} \hat{q} = -\tilde{k} \cdot \nabla T_{p_i} - p_i \left( \frac{\partial}{\partial p_i} \tilde{k} \right) \cdot \nabla T = -\tilde{k} \cdot \nabla T_{p_i} - \left( k_{ii} \frac{\partial T}{\partial x_i} \right) p_i = k_{11}, k_{22}, k_{33}.
\]  

(4.23)

The left hand side of the sensitivity equation, Eq. (4.19), can be written as:

\[
p_i \frac{\partial}{\partial p_i} \hat{e}''' = \begin{cases} \hat{e}''' & p_i = \hat{e}''' \\ 0 & \text{otherwise} \end{cases}.
\]  

(4.24)

The only time this term is non-zero is when the parameter of interest is the source term \( \hat{e}''' \).
The integral form of the sensitivity coefficient equation now becomes

$$\frac{\partial}{\partial t} \int \int (CT_{p_i} + p_i \frac{\partial C}{\partial p_i} T) d\mathcal{V} + \int \int \left[ -\kappa \cdot \nabla T_{p_i} - p_i \left( \frac{\partial}{\partial p_i} \kappa \right) \cdot \nabla T \right] \cdot d\mathcal{A} = \int \int p_i \frac{\partial \epsilon^{'''} \nu}{\partial p_i} d\mathcal{V}. \tag{4.25}$$

At this point it is appropriate to compare Eq. (4.18) and Eq. (4.25) as there are several analogous terms.

<table>
<thead>
<tr>
<th>Term</th>
<th>$T_{eqn}$</th>
<th>$T_{p_i}$ $eqn$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Capacitance</td>
<td>$CT$</td>
<td>$CT_{p_i}$</td>
</tr>
<tr>
<td>Diffusion</td>
<td>$\kappa \cdot \nabla T$</td>
<td>$\kappa \cdot \nabla T_{p_i}$</td>
</tr>
<tr>
<td>Source</td>
<td>$\epsilon^{'''}$</td>
<td>$p_i \frac{\partial \epsilon^{'''} \nu}{\partial p_i}$</td>
</tr>
</tbody>
</table>

The remaining terms in the sensitivity equation depend on temperature and not sensitivity coefficients. Consequently, if the energy equation is solved first, these remaining terms can be moved to the right hand side of the sensitivity coefficient equation. This allows the sensitivity equation to be written as

$$\frac{\partial}{\partial t} \int \int (CT_{p_i}) d\mathcal{V} + \int \int (-\kappa \cdot \nabla T_{p_i}) \cdot d\mathcal{A} = \int \int p_i \frac{\partial \epsilon^{'''} \nu}{\partial p_i} d\mathcal{V}$$

$$- \frac{\partial}{\partial t} \int \int p_i \frac{\partial C}{\partial p_i} T d\mathcal{V} + \int \int \left[ p_i \left( \frac{\partial}{\partial p_i} \kappa \right) \cdot \nabla T \right] \cdot d\mathcal{A}. \tag{4.26}$$

A very significant observation is that the left hand side of Eq. (4.26) is identical in form to the left-hand side of Eq. (4.18). Therefore, the same computer routines used for discretizing the $T$ equation can also be used for discretizing all the $T_{p_i}$ equations. This has the potential for saving code development time and computational time, particularly if the algorithm saves the global coefficient matrix associated with the discretization of the energy equation (prior to application of the boundary/initial conditions).

There are only five cases in which the right hand side of Eq. (4.26) is non-zero; these occur when $p_i = \left( \begin{array}{ccc} k_{11} & k_{22} & k_{33} \\ C & \epsilon^{'''} \end{array} \right)$. At most only one of the terms on the right hand side of Eq. (4.26) will be non-zero for a given parameter. Note that these five parameters appear explicitly in the energy equation while the remaining parameters in Eq. (4.1) appear only in the initial/boundary conditions.

Let us now look at the sensitivity coefficient initial/boundary conditions. Taking the logarithmic derivative of the initial condition, Eq. (4.11), with respect to an arbitrary parameter yields
One of the many advantages of using the scaled sensitivity coefficient is that $T_{P_o}$ has an initial condition of $T_o$ while the unscaled sensitivity coefficient has an initial condition of unity. It is much more difficult to verify the correct units of the unscaled sensitivity coefficients than the scaled sensitivity coefficients.

All three of the flux type boundary conditions have been combined into Eq. (4.16) with the boundary flux being given by Eq. (4.17). Differentiating Eq. (4.16) with respect to an arbitrary parameter and multiplying by the parameter $p_i$, we obtain:

$$\int \int \left( p_i \frac{\partial \hat{q}_b}{\partial p_i} \right) \cdot d\hat{A} \bigg|_{\hat{x}_b}^{\hat{x}_b} = \int \int p_i \frac{\partial \hat{q}_b^\prime}{\partial p_i} \cdot \hat{n} \cdot d\hat{A}.$$  

(4.28)

The integrand of the right hand side of Eq. (4.28) can be evaluated for each of the three flux type boundary conditions and are as follows:

$$p_i \frac{\partial \hat{q}_b^\prime}{\partial p_i} = \begin{cases} \hat{q}_b^\prime, & p_i = \hat{q}_b^\prime \\ 0, & \text{otherwise} \end{cases}, \text{ along } \hat{x}_b_1$$

(4.29)

$$p_i \frac{\partial \hat{q}_b^\prime}{\partial p_i} = p_i \frac{\partial \hat{q}_c^\prime}{\partial p_i} = hT_P + p_i \frac{\partial h}{\partial p_i} (T - T_{\infty}) - h_p \frac{\partial T_{\infty}}{\partial p_i}$$

$$= hT_P + \begin{cases} h(T - T_{\infty}), & p_i = h \\ -hT_{\infty}, & p_i = T_{\infty} \\ 0, & \text{otherwise} \end{cases}, \text{ along } \hat{x}_b_2$$

(4.30)

$$p_i \frac{\partial \hat{q}_b^\prime}{\partial p_i} = p_i \frac{\partial \hat{q}_r^\prime}{\partial p_i} = 4\varepsilon \sigma T^3 T_P + p_i \frac{\partial \varepsilon}{\partial p_i} \sigma (T^4 - T_r^4) - 4\varepsilon \sigma T^3 T_P \frac{\partial T_r}{\partial p_i}$$

$$= 4\varepsilon \sigma T^3 T_P + \begin{cases} \varepsilon \sigma (T^4 - T_r^4), & p_i = \varepsilon \\ -4\varepsilon \sigma T_r^4, & p_i = T_r \\ 0, & \text{otherwise} \end{cases}, \text{ along } \hat{x}_b_3$$

(4.31)

$$T_{p_i}(\hat{x}_{b_i}, t) = \begin{cases} T_b, & p_i = T_b \\ 0, & \text{otherwise} \end{cases}.$$  

(4.32)
For an isotropic material, it is not possible to simply replace $k_{ii}$ with $k$. For this case, Fourier’s Law becomes

$$\dot{q} = -k \nabla T,$$

and the following replacement must be made in Eq. (4.23):

$$k_{ii} \frac{\partial T}{\partial x_i} \Rightarrow k \nabla T.$$

All of the sensitivity coefficient equations and initial/boundary conditions are summarized in Table 4.1. The term RHS refers to the right hand side of Eq. (4.26); the left hand side has the same

| $T_{p_i}$ | RHS | $IC$ | $\frac{\partial q'''}{p_i \partial p_i} |_{x_2}$ | $\frac{\partial q'''}{p_i \partial p_i} |_{x_2}$ | $\frac{\partial q'''}{p_i \partial p_i} |_{x_2}$ | BC4 |
|---|---|---|---|---|---|---|
| $T_{k_{ii}}$ | $\int \int k_{ii} \frac{\partial T}{\partial x_i} \cdot d\mathbf{A}$ | 0 | 0 | $hT_{k_{ii}} |_{x_2}$ | $4\epsilon \sigma T^3 T_{k_{ii}} |_{x_3}$ | 0 |
| $T_k$ | $\int \int (k \nabla T \cdot d\mathbf{A})$ | 0 | 0 | $hT_k |_{x_2}$ | $4\epsilon \sigma T^3 T_k |_{x_3}$ | 0 |
| $T_C$ | $\frac{\partial}{\partial t} \int \int \int C T d\mathbf{V}$ | 0 | 0 | $hT_C |_{x_2}$ | $4\epsilon \sigma T^3 T_C |_{x_3}$ | 0 |
| $T_{\dot{e}'''}$ | $\int \int \int \dot{e}'''' d\mathbf{V}$ | 0 | 0 | $hT_{\dot{e}'''} |_{x_2}$ | $4\epsilon \sigma T^3 T_{\dot{e}'''} |_{x_3}$ | 0 |
| $T_{\dot{q}'''}$ | 0 | 0 | $\dot{q}''$ | $hT_{\dot{q}'''} |_{x_2}$ | $4\epsilon \sigma T^3 T_{\dot{q}'''} |_{x_3}$ | 0 |
| $T_h$ | 0 | 0 | 0 | $hT_h |_{x_2} + \dot{q}''$ | $4\epsilon \sigma T^3 T_h |_{x_3}$ | 0 |
| $T_c$ | 0 | 0 | 0 | $hT_c |_{x_2} + \dot{q}''$ | $4\epsilon \sigma T^3 T_c |_{x_3} + \dot{q}''$ | 0 |
| $T_{T_+}$ | 0 | 0 | 0 | $h(T_{T_+} |_{x_2} - T_\infty)$ | $4\epsilon \sigma T^3 T_{T_+} |_{x_3}$ | 0 |
| $T_{T_r}$ | 0 | 0 | 0 | $h(T_{T_r} |_{x_2} - T_r^4)$ | $4\epsilon \sigma (T^3 T_{T_r} |_{x_3} - T_r^4)$ | 0 |

**Table 4.1**: Definition of various right hand side and initial/boundary condition terms for the sensitivity coefficient equations. RHS refers to the right hand side of Eq. (4.26)
Boundary conditions require no action in an element based code. For the convective boundary condition on surface 2, all the sensitivity coefficient boundary conditions contain a term that is the product of the heat transfer coefficient times the sensitivity coefficient; those equations involving \((h, T_\infty)\) contain an additional in-homogeneous term. For the radiation boundary condition on surface 3, all of the sensitivity coefficient boundary conditions contain a homogeneous term involving the sensitivity coefficient; those involving \((\varepsilon, T_\infty)\) contain an additional inhomogeneous term.

Note that even though the original energy equation is nonlinear with a radiation boundary condition, all the sensitivity coefficient equations are linear; this has the potential for affording computational savings over the finite difference method of computing sensitivity coefficients. For the specified temperature boundary condition on surface 4, all the sensitivity coefficients have a homogeneous boundary condition, with the exception of \(T_b\).

### 5.0 Multiple Material Regions

From a practical perspective, it is desirable to be able to compute sensitivity coefficients for multiple material regions. In order to visualize the implementation steps, let us specialize the energy equation for the case of isotropic thermal conductivity for a region having two different materials. For material regions 1 and 2, we have:

\[
\frac{\partial}{\partial t} \int \int C_1 T \, dV - \int \int k_1 \nabla T \cdot \hat{n} \, dA = \int \int \hat{e}'''' \, dV \tag{5.1}
\]

\[
\frac{\partial}{\partial t} \int \int C_2 T \, dV - \int \int k_2 \nabla T \cdot \hat{n} \, dA = \int \int \hat{e}'''' \, dV . \tag{5.2}
\]
In order to determine the sensitivity coefficient for the thermal conductivity of region 1 \((k_1)\), take the derivative of Eq. (5.1) and Eq. (5.2) with respect to the \(\ln k_1\). The results are

\[
\frac{\partial}{\partial t} \int \int C_1 T_{k_1} d\psi - \int \int k_1 \nabla T_{k_1} \cdot d\hat{A} = \int \int k_1 \nabla T \cdot d\hat{A} \tag{5.3}
\]

\[
\frac{\partial}{\partial t} \int \int C_2 T_{k_1} d\psi - \int \int k_2 \nabla T_{k_1} \cdot d\hat{A} = 0. \tag{5.4}
\]

For region 1, the \(T_{k_1}\) equation has a nonzero right hand side while for region 2, the \(T_{k_1}\) equation has a zero right hand side. This is because since \(k_1\) and \(k_2\) are independent parameters, \(\partial k_2/\partial k_1 = 0\). This means that in the assembly of the \(T_{k_1}\) system of equations, one must keep track of whether you are inside or outside of region 1 and apply the appropriate equation.

The same kind of results can be developed for the volumetric heat capacity and source term sensitivity. Namely, the right-hand side contribution will be zero if you are outside the region for which the sensitivity coefficient is being computed.

### 6.0 Software Architecture

We have completed a preliminary unstructured grid software implementation for the direct differentiation method as shown in Section 4.0 for the calculation of scaled sensitivity coefficients. The implementation of the direct differentiation method is an intrusive modification to any heat conduction analysis software due to the additional sensitivity coefficient equations that need to be solved. The use of a finite difference method as discussed in Section 3.0 does not require intrusion into the analysis software when used with optimization software, see Blackwell and Eldred (1997), but has certain limitations as pointed out previously. This section will provide a brief overview of the key architectural issues and implementation methods for unstructured grid solvers. We feel that it is important to have both methods available to the analyst in order to support the use of sensitivity coefficients and uncertainty estimation during the design process.

A variety of references are available that present the architecture and implementation of unstructured grid solvers in the context of Finite Element Methods (FEM), see Hughes (1987) for a good example. Our implementation makes use of the Control Volume Finite Element Method (CVFEM) for spatial discretization and an implicit time discretization scheme, see Hogan, et al. (1996), in a multi-mechanics, unstructured grid solver called FCV. These unstructured grid methods make use of the element assembly process to arrive at the complete form of the algebraic equation for a given node point in the grid. The linear system of algebraic equations are formed by looping over all of the elements in the grid and performing a scatter-add operation from the local element matrices to the global matrix system. Boundary conditions are then applied using a loop over the Neumann type boundary conditions using a scatter-add operation, followed by the application of Dirichlet boundary conditions. This method leads naturally to an element matrix approach for both interior and boundary condition discretization. We have element level subroutines implemented for each dependent variable equation to be solved and boundary condition to
be applied. Both direct and iterative linear solvers are supported in the solver. Direct solvers are
used during development and for small-scale problems on serial compute platforms. Iterative
solvers, based on preconditioned Krylov methods, are used for large-scale serial and massively-
parallel implementations. A variety of global matrix storage methods are supported from banded
to sparse based on the linear solver requirements.

In order to support the sensitivity coefficient calculations, the key architectural feature of the
implementation is the solution driver loop in the solver. This driver loop is responsible for control-
ing the nonlinear iterations for nonlinear steady problems and time step advancement for tran-
sient problems. For nonlinear transient problems the driver loop must also control the nonlinear
iterations within the time step. In addition to handling the nonlinear and transient features of a
specific algorithm, there is a mechanism for dealing with multiple equation solutions. In general,
multiple equations can be solved in a variety of coupling methods. Fully coupled, block segre-
gated, and fully segregated methods are supported by the driver loop. This is accomplished by
introducing the concept of multiple solution phases during a step in the driver loop. Each solution
algorithm is described in a control data structure that includes the number of phases required for
each step (steady or time) and the element subroutine to assemble based on the element topology,
material model, material ID, etc. We use the term solution phase to represent each equation set
that is assembled and solved; hence the number of phases is equal to the number of equation sets
to solve. Since the total number of equations to solve for is not known until the input file is parsed,
it is this control structure which allows the solver to handle $1$ to $N$ equation solves. For heat con-
duction problems with sensitivity coefficients, we use a fully segregated approach that leads to a
total of $1 + N_p$ solution phases, where $N_p$ is the number of sensitivity coefficients requested in
the model description contained in the input file. The boundary condition application is accom-
plished by also keeping track of the current active solution phase number and applying boundary
conditions that are active for the current phase. The current phase number sets the active depen-
dent variable (or variables) that is being solved for. This dependent variable can be temperature or
any of the sensitivity coefficients shown in Table 4.1. Temperature is always solved for first, as it
is required for many of the sensitivity coefficients. In our formulation, the sensitivity coefficient
equations are linear, even if the temperature solution is nonlinear.

The complexity in dealing with the implementation of the sensitivity coefficient calculations is the
pre-processing step before the solver is applied. The current command structure in the input file is
an attempt at providing a natural form for turning on sensitivity coefficients, directed towards
uncertainty calculations. During the input file parsing, the number and type of sensitivity coeffi-
cients requested are tallied. In the case of multiple material models, the material ID is also
recorded so that the switching operation described in Section 5.0 can be accomplished during
assembly in the driver loop. Once the input file is parsed, additional boundary conditions are gen-
erated internally for each of the sensitivity coefficients to be calculated. Table 4.1 provides the
summary of boundary conditions that need to be generated for each sensitivity coefficient equa-
tion. This is accomplished by looping over each of the boundary conditions applied to the temper-
ature equation in the input file and then generating the appropriate boundary condition for the
given sensitivity coefficient equation. In many cases, the boundary conditions are zero. Boundary
conditions are segregated into Neumann and Dirichlet types by the preprocessor and the boundary
condition matrix ID is stored, along with the active solution phase number for the given boundary
condition. Initial conditions are also set for the case of the initial temperature sensitivity coeffi-
7.0 Verification Calculations

It is important to verify that computational algorithms are accurate for a problem with a known solution. We chose to look at transient heat conduction in a two-dimensional rectangular region with an orthotropic thermal conductivity. This problem is shown in Figure 7-1 and has an analytical solution developed by Dowding (1996). A heat flux is applied over one third of the lower face parallel to the x-axis. All other surfaces are adiabatic. The cross section is 7.62 cm by 1.0 cm. The thermal conductivity tensor is orthotropic with the principal direction aligned with the coordinate axes. This problem was chosen to demonstrate that the two conductivity sensitivity coefficients behave differently and verify the numerical computation of temperature and sensitivity coefficients.

Thermal properties selected for the problem, and listed in Figure 7-1, are representative of carbon-carbon composite (Dowding, et al., 1996). This particular composite has a ratio for the orthotropic thermal conductivity of 15. The physical aspect ratio of the problem is 7.62/1, but because the thermal conductivity is much larger in the x-direction, the thermal aspect ratio which accounts for the difference in thermal conductivity is approximately 2 (7.62/1.2/45 = 2). For this reason,
the ratio of the number of elements in the principal directions is two (a mesh refinement is investigated later). Contour plots of the temperature and sensitivity coefficients, for both components of thermal conductivity and the volumetric heat capacity, are shown in Figure 7-2. The heat flux has been applied for 20 seconds beginning at a uniform initial temperature of 30 °C.

The temperature (and its gradient) is largest at the corner of the body where the heat flux is applied. Magnitudes of the sensitivity coefficients are also largest in this region for all coefficients. Sensitivities for the two components of thermal conductivity \((k_x, k_y)\) are quite different. The sensitivity to \(k_x\) changes sign traversing the body in the y-direction, while a sign change occurs in the x-direction for the sensitivity to \(k_y\). At intermediate locations, the sensitivities have a zero magnitude. The location of the zero sensitivity coefficient moves around with time. It is fairly

---

**FIGURE 7-2** Contour plots for the temperature and sensitivity coefficients throughout the spatial region for the verification problem with orthotropic thermal conductivity problem after heating for 20 seconds.
common for the thermal conductivity sensitivity coefficients to go through a sign change for problems with a specified flux.

The volumetric heat capacity sensitivity is negative throughout the problem domain, consistent with the fact that increasing the heat capacity decreases the temperature. The volumetric heat capacity sensitivity is much more uniform than either of the thermal conductivity sensitivities. The farther one goes away from the location where the heat flux is applied, the smaller the magnitude of the volumetric heat capacity sensitivity coefficient.

Although contour plots are beneficial for visualizing the spatial variation, a standard xy-plot is useful for comparing numerical computations to analytical values and seeing specific magnitudes. Temperatures and sensitivity coefficients along the top and bottom faces (planes y = 0 and y = 0.01 m) are shown in Figure 7-3 after applying the heat flux for \( t = 20 \) seconds. For these computations a mesh with 30 elements in the x-direction and 15 elements in the y-direction is used with a time step of 0.5 seconds. The difference between the numerical results and analytical results are not discernible in this figure. Hence, adding additional numerical values for a refined mesh will not demonstrate the accuracy. It is more appropriate to look at the difference between numerical and analytical values. Using the definition of relative error in Eq. (3.3) the errors in the computation of temperature and sensitivity were computed by comparing to the analytical solution. The results are shown in Figure 7-4. Two refinements of the mesh are shown. In each refinement the number of nodes in the two directions was doubled, while the time step was reduced by a factor of four. The mesh scale Fourier number was \( \alpha_x \Delta t / \Delta x^2 = 2.325 \) and \( \alpha_y \Delta t / \Delta y^2 = 2.25 \) for all calculations. All of the error results demonstrate second order spatial accuracy as the mesh is refined.

8.0 Acknowledgments

The authors would like to acknowledge discussions relative to sensitivity coefficients with Professor A. Emery of the University of Washington and T. Fadale, Applied Research Associates. Also, we would like to acknowledge Professor J. V. Beck of Michigan State University for having introduced us to the useful concept of sensitivity coefficients.

9.0 References


FIGURE 7-3 Computed temperature (rise) and sensitivity coefficients along the $y=0$ and $y=0.01m$ plane for orthotropic verification problem at $t=20$ seconds.
\begin{figure}
\centering
\includegraphics[width=\textwidth]{figure7-4.png}
\caption{Relative error at location of maximum temperature rise \((x=0, y=0)\) as a function of the number of elements.}
\end{figure}


