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Sensitivity and Uncertainty Analysis for Thermal Problems

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ABSTRACT

A discussion of various methods used to compute sensitivity information is presented. The methods include differentiation of analytical solutions, finite difference, complex step, software differentiation, sensitivity equation method, and adjoint methods. Example calculations are presented for several of these methods. It is emphasized that sensitivity information is important in its own right as opposed to simply being one of the many ingredients necessary to perform parameter estimation and/or optimization calculations. Strengths and weaknesses of the various sensitivity methods are discussed.

NOMENCLATURE

A	area, m^2
C	$= \rho c_p$, volumetric heat capacity, J/m^3-K
c_p	specific heat, J/kg-K
h	convective heat transfer coefficient, W/m^2-K
k	thermal conductivity, W/m-K
[K]	global conduction matrix
L	thickness of slab, m
n_p	number sensitivity coefficients (parameters)
n_s	number of sensors
$\{p\}$	parameter vector
p_i	element of $\{p\}$
q	heat flux, W/m^2
T	temperature, K
T_p	scaled sensitivity coefficient, $= p\partial T/\partial p$
t	time, s
α	thermal diffusivity, m^2/s
ε	emittance
σ	Stefan-Boltzmann constant

INTRODUCTION

When analyzing the response of a thermal system, a large number of parameters must be specified to characterize the system. These parameters include material properties (density, specific heat, thermal conductivity, emittance, etc.), geometry, and boundary conditions (heat flux, convective heat transfer coefficient, etc.). During the design phase of a project, some of the parameters may change as the design evolves. In many instances, these parameters are not known with a high degree of precision. Also, a designer may be free to choose among many different competing materials. As an example, a design might call for 304 stainless steel; alternative stainless steels such as 316 might work equally well and could be used interchangeably (depending on availability). Even if we consistently use 304 stainless, there may be manufacturer-to-manufacturer variability as well as lot-to-lot variability from a single manufacturer. Consequently, we need to play "what if" scenarios with regard to the material properties in order to assure ourselves that the lot-to-lot or manufacturer-to-manufacturer variability does not produce undesirable consequences.

Historically, these "what if" scenarios have been performed on an ad hoc basis; selected parameter values would be changed and the analysis repeated. Without the aid of a computer, only a limited number of parameter studies could be performed. However, today's computers now make it possible to perform a wide range of parameter studies. Even with the computer, these parameter studies still tend to be performed on an ad hoc basis. Based on a designer's intuition, the most important parameters would be varied over some range. Since intuition is only as good as prior experiences, it is possible for even an experienced designer or analyst to miss an important parameter. It is also time consuming to study parameters in an ad-hoc manner. Consequently, a more formal procedure needs to be developed. This is where *sensitivity analysis* plays an important role.

A desirable goal of the design process is to produce *robust designs* that can reliably function

over a wide range of operating conditions. This is particularly true for mission critical components. For example, the on-board flight controller for a rocket system must be capable of functioning when the ambient temperatures range from high altitude space to desert launch pad. Is it possible for the hardware to operate if the system parameters differ from the nominal values assumed in the analysis phase? The robustness of a design can be investigated by means of a *sensitivity analysis*.

Sensitivity analysis is defined as the study of how variations in input parameters of a computational model cause variations in output. Input parameters would include material properties, boundary/initial conditions, and geometry; output variables might be displacement, stress and/or temperature. A measure of this sensitivity is termed the sensitivity coefficient and is (mathematically) defined as the partial derivative of the output variable with respect to the parameter of interest. For a general discussion of sensitivity coefficients, see Beck and Arnold [1] and Beck, et al. [2]. Since the focus of this work is on thermal problems, let us define the first order sensitivity coefficient of the temperature field with respect to the thermal conductivity k as

$$\text{thermal conductivity sensitivity coefficient} = \frac{\partial}{\partial k} T(\hat{x}, t; k) \qquad (1)$$

where it is understood that all parameters other than thermal conductivity are held fixed during the differentiation. The sensitivity coefficient is also a field variable in that it depends on position and time just like temperature. In order to understand how one might use the sensitivity coefficient to predict how a system responds if you perturb the thermal conductivity, let us expand the temperature field in a Taylor series about the mean value of the thermal conductivity

$$T(\hat{x}, t; k) = T(\hat{x}, t; \bar{k}) + \left.\frac{\partial T}{\partial k}\right|_{\bar{k}} (k - \bar{k}) + \left.\frac{1}{2}\frac{\partial^2 T}{\partial k^2}\right|_{\bar{k}} (k - \bar{k})^2 + \ldots \qquad (2)$$

From this expansion, one can see how the first order sensitivity coefficient is needed for a first order analysis and higher order sensitivity coefficients are required for higher order analysis. This work will focus on first order sensitivity analysis as the computational load scales approximately linearly with the number of parameters. For a second order analysis, the computational load scales as the square of the number of parameters; this may become prohibitive for problems with hundreds of parameters. If the system response and first order sensitivity coefficients are known for the nominal parameter values, Eq. (2) (with higher order terms neglected) can be used to compute the response at a neighboring point in parameter space. If higher order sensitivity coefficients are required, an initial approach might be to compute second order sensitivity coefficients only for those selected parameters that have large first order sensitivity coefficients.

In some cases, only the sign of the sensitivity coefficient is important. If for example, the length of a system is increased, does the critical temperature go up or down?

In many instances, the sensitivity coefficient is often required as an intermediate step in the solution of parameter estimation, function estimation, uncertainty propagation, and optimization problems. The emphasis of this work is on calculating sensitivity coefficients because they have importance themselves as opposed to just numbers that are fed into a parameter estimation or optimization process.

SUMMARY OF METHODS FOR COMPUTING SENSITIVITY COEFFICIENTS

Sensitivity coefficients can be calculated by many methods. These methods include the following:

- differentiation of analytical solutions
- finite difference
- complex step
- software differentiation (e.g. ADIFOR/ ADIC)
- sensitivity equation method
- adjoint methods

Each of these methods has it place. In many instances, multiple methods will be used on the same problem to verify that the primary method produces the desired results. Example calculations will be presented for most of these methods.

DIFFERENTIATION OF ANALYTICAL SOLUTIONS

Differentiation of analytical solutions is probably the simplest method. It involves differentiating an analytical solution with respect to the parameter(s) of interest. If the analytical expressions are very complex, then symbolic algebra programs such as Mathematica®, Maple®, Macsyma®, etc. will prove invaluable. Obviously, this approach is limited to problems in which analytical solutions are available; this severely limits the problems which can be addressed by this method. Recent work by McMasters, et al. [3] using Green's functions has produced software

that will provide and evaluate analytical solutions for a wide variety of 3-D time dependent heat conduction problems in rectangular geometries. It has been the author's experience that one of the most significant uses of this method is to serve as a tool to verify other approximate numerical methods.

As an example of this method, consider a 1-d

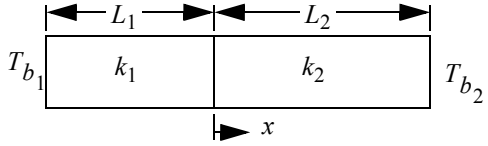


Figure 1. Problem definition for 1-D two layer slab problem.

configuration that might be used in the comparative method for the determination of thermal conductivity. This geometry is shown in Fig. 1. Fixed boundary temperatures are applied on the two ends and the steady state temperature profile is measured. The conductivity of one specimen is known and the other is to be determined. The analytical expressions for the temperature profile are

$$T_1(x) = \frac{k_1L_2T_{b_1} + k_2L_1T_{b_2}}{k_1L_2 + k_2L_1} - \frac{k_2L_1(T_{b_1} - T_{b_2})}{k_1L_2 + k_2L_1}\frac{x}{L_1} \quad (3)$$

$$T_2(x) = \frac{k_1L_2T_{b_1} + k_2L_1T_{b_2}}{k_1L_2 + k_2L_1} - \frac{k_1L_2(T_{b_1} - T_{b_2})}{k_1L_2 + k_2L_1}\frac{x}{L_2}. \quad (4)$$

In the design of this experiment, one would like to have a large sensitivity to the unknown thermal conductivity and a small sensitivity to the known thermal conductivity. The two thermal conductivity sensitivity coefficients can be computed analytically and are given by

$$k_1\frac{\partial T_1}{\partial k_1} = T_{k_1} = \frac{k_1L_2k_2L_1}{(k_1L_2 + k_2L_1)^2}(T_{b_1} - T_{b_2})\left(1 + \frac{x}{L_1}\right), \quad (5)$$

$$T_{k_1} = -T_{k_2}, \quad -L_1 \le x \le 0$$

$$k_1\frac{\partial T_1}{\partial k_1} = T_{k_1} = \frac{k_1L_2k_2L_1}{(k_1L_2 + k_2L_1)^2}(T_{b_1} - T_{b_2})\left(1 - \frac{x}{L_2}\right), \quad (6)$$

$$T_{k_1} = -T_{k_2}, \quad 0 \le x \le L_2.$$

The temperature and conductivity sensitivity coefficient profiles are shown in Fig. 2. Each profile consists of two straight line segments. The sensitivity coefficient T_{k_1} is positive throughout, which indicates that increasing k_1 increases the

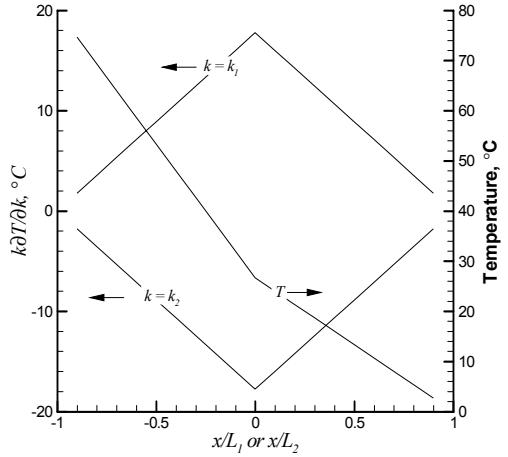


Figure 2. Temperature profile and conductivity sensitivity coefficients for two layer slab problem.

temperature. The sensitivity coefficient T_{k_2} is negative throughout, which indicates increasing k_2 decreases the temperature. The location of maximum thermal conductivity sensitivity T_{k_1} is at the interface between the two regions. This might seem strange at first, but remember that the conductivity sensitivity is identically zero on the boundaries and positive in between. Consequently, this forces the maximum sensitivity to be at an interior point. Note that the two conductivity sensitivity coefficients are correlated. This means that from a parameter estimation perspective, you can not estimate both thermal conductivities from the same experiment. Hence, the name comparator is appropriate.

The above sensitivity coefficients can be used to choose the specimen lengths as well as sensor locations.

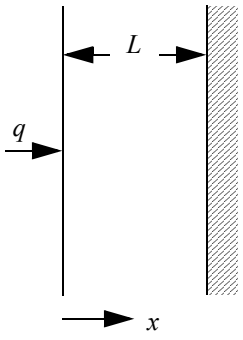
FINITE DIFFERENCE DETERMINATION OF SENSITIVITY COEFFICIENTS

If a sensitivity analysis requires an analytical solution, then we would be severely limited in the problems that we can address. Fortunately, general purpose software is available to numerically solve complex three dimensional, time dependent thermal problems. The discretization schemes include finite difference, finite volume, control volume finite element and finite element methods. In industry, commercially available software is often used and source code is generally not available. For this case, sensitivity coefficients are often computed by running the software for two different values of a parameter and using a first order forward difference. Scaled sensitivity coefficients are then determined from

$$T_{p_i} = p_i[T(p_1, p_2, \ldots, p_i + \Delta p_i, \ldots, p_n) - T(p_1, p_2, \ldots, p_i, \ldots, p_n)]/\Delta p_i + O(\Delta p_i). \quad (7)$$

This approach requires n+1 solutions for the temperature field and will be first order accurate in Δp_i. If a second order accurate central difference is used instead, 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 you numerically solve the problem with different inputs. Since no source code modification is required, the software development costs for this method will be minimal. Commercial software can be used to accomplish this, provided the computational results are available with sufficient precision.

Some numerical experimentation is strongly recommended to determine an acceptable value for the finite difference step size Δp. 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 one dimensional, constant flux problem given in Fig. 3. This example was



$q = 4\text{x}10^5$ W/m^2
$k = 10$ W/m-K
$L = 0.01$ m
$T_o = 300$ K
$\rho = 8000$ kg/m^3
$c_p = 500$ J/kg-K
$\alpha = 2.5\text{x}10^{-6}$ m^2/s
$qL/k = 400$ K
adiabatic back wall

Figure 3. Schematic of constant heat flux problem for 1-d planar slab.

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 significant digits) was utilized. The final problem time was 20 s, which corresponded to a dimensionless time $\alpha t/L^2 = 0.5$. The dimensionless thermal conductivity sensitivity coefficient at $x = 0$ and $t = 20$ s was computed, utilizing a range of values for Δk for a forward difference approximation. The relative error in each computation was computed from

$$\%\ \text{Error} = 100\frac{T_{k_n} - T_{k_a}}{T_{k_a}} \quad (8)$$

where the subscripts n and a represent numerical and analytical, respectively; the error results are presented in Fig. 4. Uniform grids of 10 and 20

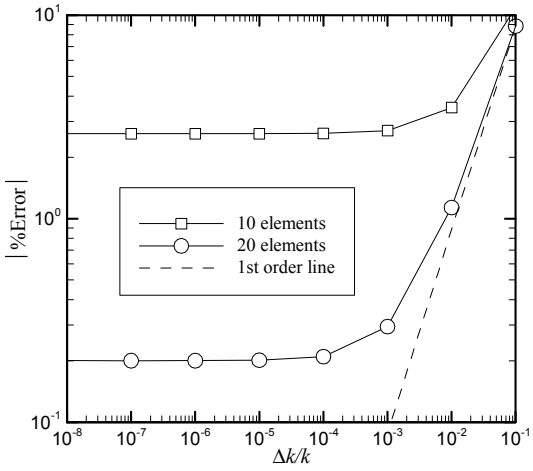


Figure 4. Thermal conductivity sensitivity coefficient errors at $x = 0$ and $t = 20$ s as a function of $\Delta k/k$ for two grid refinements.

elements were used along with a fixed grid scale Fourier number ($\alpha\Delta t/\Delta x^2 = 5$). Focusing on the upper right hand corner of this figure, 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 approximation to the sensitivity coefficient (forward difference) would decay linearly with decreasing finite difference step size. However, there are additional discretization errors in the numerically generated temperature field. The curve in Fig. 4 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. This is particularly noticeable for the 10 element case. 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. If the finite difference step size is made even smaller, it is possible that the errors will become even larger. An example of this behavior is shown in the next section.

COMPLEX STEP METHOD

The main criticism of the *finite difference method* for computing sensitivity coefficients is that the computational results exhibit a step size dependence. In practice, this means that for each (class of) problem(s), one needs to perform a step size parameter study for each sensitivity coefficient. Unfortunately, this could be a time consuming process for practical problems with

ten's of parameters. The *complex step method* offers a practical method of eliminating the step size dependence of finite difference methods, but at the expense of software modification and increased run time.

The derivation of the complex step method follows from a Taylor series expansion of the real valued function f about the complex (imaginary) parameter value $p + i\Delta p$ with $i = \sqrt{-1}$. This series is

$$f(p + i\Delta p) = f(p) + \left.\frac{\partial f}{\partial p}\right|_p i\Delta p - \frac{1}{2!}\frac{\partial^2 f}{\partial p^2}\Delta p^2 - \frac{1}{3!}\frac{\partial^3 f}{\partial p^3} i\Delta p^3 + O(\Delta p^4). \quad (9)$$

Taking the imaginary part of Eq. (9), one obtains

$$Im[f(p + i\Delta p)] = \left.\frac{\partial f}{\partial p}\right|_p \Delta p - \frac{1}{3!}\frac{\partial^3 f}{\partial p^3}\Delta p^3 + \ldots . \quad (10)$$

Solving for the first derivative yields

$$\left.\frac{\partial f}{\partial p}\right|_p = \frac{Im[f(p + i\Delta p)]}{\Delta p} + O(\Delta p^2) . \quad (11)$$

This simple result says that the derivative of the function is obtained by taking the *imaginary* part of the complex function $f(p + i\Delta p)$ divided by the real parameter step size Δp. Note that this result is second order accurate while Eq. (7) is first order accurate. Computational results for the complex step method have been presented by Martins, et al. [4]; they have applied the method to both analytical expressions as well as multidimensional structural and fluid dynamic codes. They demonstrated that the step size can be made arbitrarily small without suffering the loss of accuracy associated with the finite difference method. However, this result comes at the expense of code modification and increased run times

The computational procedure is as follows: 1) in the source code, declare all parameter values and the function f to be complex variables; 2) for the parameter p of interest, replace p by $p + i\Delta p$ in the input; 3) execute the software to compute f as a complex variable; 4) evaluate Eq. (11) for the sensitivity coefficient for parameter p. The process outlined above must be repeated for each parameter. Hence, the process of generating multiple sensitivity coefficients is similar to that for the *finite difference method* in that multiple runs of the same software are required. However, the big difference is that the step size Δp in Eq. (11) can be set to roughly machine zero and the results will be independent of step size. The *complex step method* will eliminate the (generally annoying) step of a parametric study in step size.

The complex step method has been applied to the same example considered in DIFFERENTIATION OF ANALYTICAL SOLUTIONS and the results are given in Fig. 5.

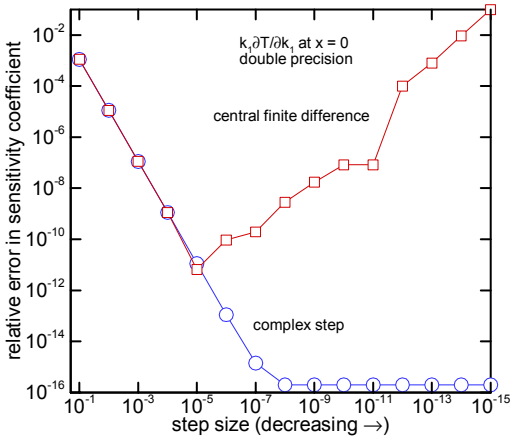


Figure 5. Relative error in conductivity sensitivity coefficient as a function of finite difference step size.

For comparison purposes, the central finite difference results are also shown. Both methods are second order accurate in the finite difference step size. Therefore, one would expect similar accuracy provided there are no machine precision problems. Both methods display second order behavior for step sizes down to 10^{-5}, as evidenced by the straight line behavior with a slope of -2. Further reductions in step size below 10^{-5} cause the central difference method errors to increase. Contrast this with the complex step method which is capable of driving the errors to machine zero. Although there may be a wide range of step sizes for which the central difference method produces acceptable accuracy, one is never sure what this range might be for a different problem. The rule of thumb on step size that is given in Nocedal and Wright [5] suggested that $2\text{x}10^{-11}$ would be appropriate for a central difference. For this problem, it appears that this rule of thumb is optimistic.

The authors have also applied the *complex step method* to a finite volume heat conduction code and computed sensitivity to multiple thermal conductivities and a contact conductance. References [6]-[9] apply the *complex step method* to compute sensitivity coefficients for a variety of aerodynamic problems. Some computational aids for converting a code from real to complex can be found in Reference [10].

SOFTWARE DIFFERENTIATION

The software differentiation method is a recent

development. An existing source code (FORTRAN 77 or C) is input into a special pre-processor (ADIFOR or ADIC) that performs line-by-line differentiation of the original source code while producing a new source code for the sensitivity coefficient. Examples of this technology are presented by Bischof, et al. [11], where they have successfully applied it to large codes. If there are multiple parameters for which sensitivity is desired, multiple runs of the pre-processor ADIFOR or ADIC are required. If the original source code is modified (enhancements, bug fixes, etc.), then the pre-processor must be run again. Since our work has been focused primarily on techniques that can be readily applied to software under development as well as many parameter problems, we have not personally exercised the software differentiation methods.

SENSITIVITY EQUATION METHOD

A sensitivity coefficient is a field variable just like temperature and will have its own describing equation. In this section, we will demonstrate how to derive the field equation(s) for sensitivity coefficients; this method is termed the *Sensitivity Equation Method* (SEM). This process involves the differentiation of the describing equation, along with associated initial/boundary conditions, with respect to the parameters of interest. These sensitivity equations are then solved numerically, using the same kind of algorithm as is used to solve the energy equation. To demonstrate this process, consider a 1-D planar slab with a radiation boundary condition on one face and convection boundary condition on the other face; this problem is shown schematically in Fig. 6. Due

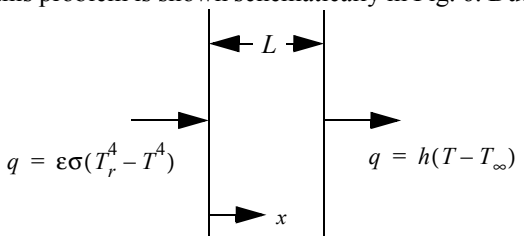


Figure 6. Schematic of 1-D problem with radiation and convection boundary conditions.

to the nonlinear radiation boundary condition, this problem is unlikely to have an exact analytical solution. Hence, a numerical solution will be explored. The energy equation and boundary conditions can be written as follows:

$$C\frac{\partial T}{\partial t} + \frac{\partial q}{\partial x} = 0 \tag{12}$$

$$q = -k\frac{\partial T}{\partial x} \tag{13}$$

$$q\big|_{x=0} = -k\frac{\partial T}{\partial x}\bigg|_{x=0} = \varepsilon\sigma(T_r^4 - T^4)\big|_{x=0} \tag{14}$$

$$q\big|_{x=L} = -k\frac{\partial T}{\partial x}\bigg|_{x=L} = h(T - T_\infty)\big|_{x=L} \tag{15}$$

$$T(x, 0) = T_i\,. \tag{16}$$

The parameters for this problem are given by the vector

$$\{p\}^T = \{C \;\; k \;\; \varepsilon \;\; T_r \;\; h \;\; T_\infty\}^T \tag{17}$$

Now, we differentiate Eq. (12)-Eq. (16) with respect to each element in the parameter vector, Eq. (17). Starting with the volumetric heat capacity sensitivity coefficient, we will differentiate Eq. (12) with respect to C, resulting in

$$\frac{\partial}{\partial C}\left(C\frac{\partial T}{\partial t}\right) + \frac{\partial}{\partial C}\left(\frac{\partial q}{\partial x}\right) = C\frac{\partial}{\partial t}\left(\frac{\partial T}{\partial C}\right) + \frac{\partial T}{\partial t} + \frac{\partial}{\partial x}\left(\frac{\partial q}{\partial C}\right) = 0 \tag{18}$$

where it has been assumed that the order of differentiation can be interchanged. Again, we will introduce the scaled sensitivity coefficient by multiplying Eq. (18) through by C to obtain

$$C\frac{\partial}{\partial t}\left(C\frac{\partial T}{\partial C}\right) + C\frac{\partial T}{\partial t} + \frac{\partial}{\partial x}\left(C\frac{\partial q}{\partial C}\right) = 0\,. \tag{19}$$

The volumetric heat capacity sensitivity coefficient is readily identified in Eq. (19). The sensitivity of the heat flux to changes in the volumetric heat capacity can be determined by differentiating Fourier's Law with respect to C, resulting in

$$q_C = C\frac{\partial q}{\partial C} = -k\frac{\partial}{\partial x}\left(C\frac{\partial T}{\partial C}\right) = -k\frac{\partial T_C}{\partial x}\,. \tag{20}$$

Eq. (19) can now be written as

$$C\frac{\partial T_C}{\partial t} - \frac{\partial}{\partial x}\left(k\frac{\partial T_C}{\partial x}\right) = -C\frac{\partial T}{\partial t}\,. \tag{21}$$

Eq. (19) is the partial differential equation that describes the field variable T_C. Note that the left hand side of this equation is identical in form to that of the original energy equation. However, there is an apparent source term on the right hand side that was not present in the energy equation. If the temperature field is known, then this source term is a known function of position and time.

We will continue the development of the equations governing the behavior of T_C by differentiating the initial/boundary conditions with

respect to C. Evaluating Eq. (20) at the $x = 0$ boundary and differentiating Eq. (14) with respect to C, this boundary condition becomes

$$C\frac{\partial q}{\partial C}\bigg|_{x=0} = -k\frac{\partial T_C}{\partial x}\bigg|_{x=0} = -4\varepsilon\sigma T^3 T_C\big|_{x=0}. \quad (22)$$

While the left hand side boundary condition for the energy equation was nonlinear and inhomogeneous, the corresponding T_C boundary condition is *linear* and *homogeneous*. This assumes again that the temperature field is known prior to the computation of the sensitivity field. Through a similar procedure, the boundary condition for the right face is given by

$$C\frac{\partial q}{\partial C}\bigg|_{x=L} = -k\frac{\partial T_C}{\partial x}\bigg|_{x=L} = hT_C\big|_{x=L}. \quad (23)$$

This boundary condition is linear and homogeneous. Since the initial condition is independent of the volumetric heat capacity, the corresponding sensitivity initial condition is the zero condition

$$C\frac{\partial T}{\partial C}\bigg|_{x,0} = T_C\big|_{x,0} = 0. \quad (24)$$

The formulation of the field equation and associated boundary/initial conditions for T_C is complete and is given by Eq. (20)-Eq. (24). Due to the similarities in form of the energy equation and the volumetric heat capacity sensitivity equation, the same technique can be used to numerically solve these equations. It does not matter if the discretization algorithm is finite difference, finite volume, control volume finite element or finite element. In fact, the existing software coding used to include the effects of capacitance, diffusion and source terms for the energy equation can be used to form the analogous terms for the sensitivity equation. The computational procedure is to first time march the energy equation one time step and then solve the sensitivity equation. The source term for T_C in Eq. (21) is known from the temperature solution. Even though the original energy equation was nonlinear because of the radiation boundary condition, the corresponding sensitivity equation is a *linear* equation. This linearity may afford computational savings, depending on the algorithm used to solve the nonlinear algebraic equations resulting from the discretization of the energy equation.

From Eq. (21), *the time rate of change of temperature drives the volumetric heat capacity sensitivity field*. If the temperature field is not changing with time, the volumetric heat capacity sensitivity will tend toward zero. For a problem with a positive temperature rise rate, this source term is negative, suggesting a negative sensitivity to the volumetric heat capacity. Similarly, for a body that is cooling, the source term is positive which suggests a positive sensitivity to the volumetric heat capacity. As one can see, insight into the thermal response can be gained by simply studying the describing equation for the sensitivity coefficients. In some cases, trends may be determined without actually solving the sensitivity equations. However, it is best to continue the process and numerically solve the sensitivity equations in order to gain maximum insight.

Next, we will derive the equation for the thermal conductivity sensitivity. The thermal conductivity sensitivity equation will be more complicated because thermal conductivity appears in both the differential equation and boundary conditions. Following the same procedure as above, the differential equation for T_k can be written as

$$C\frac{\partial}{\partial t}\left(k\frac{\partial T}{\partial k}\right) + \frac{\partial}{\partial x}\left(k\frac{\partial q}{\partial k}\right) = C\frac{\partial T_k}{\partial t} + \frac{\partial q_k}{\partial x} = 0. \quad (25)$$

Differentiating Fourier's Law with respect to thermal conductivity k, we obtain

$$q_k = k\frac{\partial q}{\partial k} = -k\frac{\partial T_k}{\partial x} - k\frac{\partial T}{\partial x}. \quad (26)$$

While Fourier's Law involves a single term, the sensitivity of Fourier's Law with respect to the thermal conductivity involves two terms. The first term involves what can be thought of as a flux of sensitivity information plus a second term that is the heat flux itself. Combining Eq. (25) and Eq. (26), the T_k equation becomes

$$C\frac{\partial T_k}{\partial t} - \frac{\partial}{\partial x}\left(k\frac{\partial T_k}{\partial x}\right) = \frac{\partial}{\partial x}\left(k\frac{\partial T}{\partial x}\right) = -\frac{\partial q}{\partial x}. \quad (27)$$

Again, the left hand side of the T_k equation is identical in form to the energy equation; the right hand side has a fictitious source term that is equal to the negative of the gradient of the heat flux. *Gradients in local heat flux drive the thermal conductivity sensitivity field.*

Care must be exercised in deriving the boundary conditions for the T_k equation. Intuitively, one might be inclined to derive a boundary condition on $k\partial T_k/\partial x$. However, we need a condition on q_k which can simply be derived by differentiation of the right hand sides of Eq. (14) and Eq. (15) with respect to the thermal conductivity. The results are

$$q_k\big|_{x=0} = k\frac{\partial q}{\partial k}\bigg|_{x=0} = -4\varepsilon\sigma T^3 T_k\big|_{x=0} \quad (28)$$

$$q_k\big|_{x=L} = k\frac{\partial q}{\partial k}\bigg|_{x=L} = hT_k\big|_{x=L}. \qquad (29)$$

Again, the nonlinear, inhomogeneous boundary condition for the energy equation has become a linear, homogeneous boundary condition for the thermal conductivity sensitivity equation, provided the temperature field is known. The initial condition simply becomes

$$k\frac{\partial T}{\partial k}\bigg|_{x,0} = T_k\big|_{x,0} = 0. \qquad (30)$$

The only inhomogeneous term in the thermal conductivity sensitivity equation is the gradient of heat flux term on the right hand side of the T_k equation in Eq. (27).

We have addressed two of the three gradient type boundary conditions that commonly occur. The third type of gradient boundary condition is a specified heat flux. This kind of boundary condition can occur, for example, when there is an electric heater present. Since the magnitude of a specified flux is independent of either the thermal conductivity or the volumetric heat capacity, this boundary condition becomes "adiabatic like"

$$\frac{\partial T_C}{\partial x}\bigg|_b = q_k\big|_b = 0 \qquad (31)$$

where the subscript b designates the generic boundary along which this boundary condition is applied. Note that for the thermal conductivity sensitivity coefficient, $\partial T_k/\partial x \neq 0$ along a specified flux boundary. This is a subtle point that requires careful thought.

The last boundary condition type that we will address is the specified temperature boundary condition. Again, since this is an imposed boundary condition that is independent of volumetric heat capacity or thermal conductivity, specified temperature boundary conditions become specified sensitivity coefficient boundary conditions with a value of zero.

$$T_C\big|_b = T_k\big|_b = 0, \text{ along specified T boundaries} \qquad (32)$$

Of the parameters listed in Eq. (17), the thermal conductivity k and volumetric heat capacity C are special in that they both appear in the describing differential equation. For their respective sensitivity describing equation, inhomogeneous terms are present. For all other parameters that do not appear in the energy differential equation, their sensitivity describing equation can be written as

$$C\frac{\partial T_p}{\partial t} - \frac{\partial}{\partial x}\left(k\frac{\partial T_p}{\partial x}\right) = 0, p \neq k, C \qquad (33)$$

where T_p is the sensitivity coefficient for parameter p; note that this is a homogeneous equation.

The boundary conditions for the four remaining parameters in Eq. (17) will now be addressed. Differentiating the $x = 0$ boundary condition given by Eq. (14) with respect to these parameters results in

$$\varepsilon\frac{\partial q}{\partial \varepsilon}\bigg|_{x=0} = \varepsilon\left[\sigma(T_r^4 - T^4) - 4\varepsilon\sigma T^3\frac{\partial T}{\partial \varepsilon}\right]\bigg|_{x=0} \qquad (34)$$
$$= [\varepsilon\sigma(T_r^4 - T^4) - 4\varepsilon\sigma T^3 T_\varepsilon]\big|_{x=0}$$

$$\Delta T_r\frac{\partial q}{\partial T_r}\bigg|_{x=0} = \Delta T_r\left[4\varepsilon\sigma T_r^3 - 4\varepsilon\sigma T^3\frac{\partial T}{\partial T_r}\right]\bigg|_{x=0} \qquad (35)$$
$$= 4\varepsilon\sigma(T_r^3\Delta T_r - T^3 T_{T_r})\big|_{x=0}$$

$$h\frac{\partial q}{\partial h}\bigg|_{x=0} = h\left(-4\varepsilon\sigma T^3\frac{\partial T}{\partial h}\right)\bigg|_{x=0} = -4\varepsilon\sigma T^3 T_h\big|_{x=0} \qquad (36)$$

$$\Delta T_\infty\frac{\partial q}{\partial T_\infty}\bigg|_{x=0} = \Delta T_\infty\left(-4\varepsilon\sigma T^3\frac{\partial T}{\partial T_\infty}\right)\bigg|_{x=0} \qquad (37)$$
$$= -4\varepsilon\sigma T^3 T_{T_\infty}\big|_{x=0}$$

Rather than using T_r and T_∞ to scale their respective sensitivity coefficients, a temperature change ΔT_r or ΔT_∞ is used. This eliminates problems with zero temperature when absolute temperature units are not used. These reference temperature changes represent a characteristic temperature change for the problem. As an example, one might choose the maximum temperature rise of the system, T_{max} - T_i. The same reference temperature rise could be used for both T_r and T_∞ sensitivities, although this is not necessary. Since the describing equation is homogeneous for those parameters that do not appear in the energy equation, the inhomogeneities in the boundary or initial conditions will drive the remaining sensitivities. For example, the emissivity sensitivity is driven in Eq. (34) by the radiative heat flux term $\varepsilon\sigma(T_r^4 - T^4)$.

By now, one should see a pattern developing in the sensitivity equations. With this in mind, the remaining results will be given as

$$\varepsilon\frac{\partial q}{\partial \varepsilon}\bigg|_{x=L} = hT_\varepsilon\big|_{x=L} \qquad (38)$$

$$\Delta T_r \left.\frac{\partial q}{\partial T_r}\right|_{x=L} = hT_{T_r}\Big|_{x=L} \tag{39}$$

$$h\left.\frac{\partial q}{\partial h}\right|_{x=L} = [h(T-T_\infty)+hT_h]\Big|_{x=L} \tag{40}$$

$$\Delta T_\infty \left.\frac{\partial q}{\partial T_\infty}\right|_{x=L} = h(T_{T_\infty}-\Delta T_\infty)\Big|_{x=L}. \tag{41}$$

The inhomogeneities in the h and T_∞ sensitivity boundary conditions at $x = L$ are the convective heat fluxes $h(T-T_\infty)$ and $h\Delta T_\infty$ respectively.

We have discussed the initial conditions for both T_C and T_k, Eq. (24) and Eq. (30) respectively; they are both zero. It is easy to see that if the parameter of interest is anything other than the initial temperature itself, the initial condition for T_p will be zero. The initial conditions can be summarized as follows:

$$p_i \left.\frac{\partial T}{\partial p_i}\right|_{x,\,0} = T_{p_i}\Big|_{x,\,0} = \begin{pmatrix} 0, p_i \neq T_i \\ \Delta T_i, p_i = T_i \end{pmatrix}. \tag{42}$$

As with other sensitivity coefficients related to temperature, we have used a temperature change as a scale factor.

After the implementation of the sensitivity equations, the first step is to perform verification calculations to insure that the equations are being solved correctly. Since we already have evaluated the analytical solution for the problem described in Fig. 3, we will repeat the solution to this problem using a control volume finite element method with a lumped capacitance and fully implicit time integration scheme. We will compute a percent error as a function of a grid metric using Eq. (8). This will allow one to verify that the order of convergence of the scheme as the grid is refined. All calculations were performed with a fixed grid scale Fourier number ($\alpha\Delta t/\Delta x^2 = 5.0$). We focus on the spatial location $x = 0$ for times of 4 s ($\alpha t/L^2 = 0.1$) and 20 s ($\alpha t/L^2 = 0.5$). The grid refinement results are shown in Fig. 7. The 4 s results are all less accurate than the 20 s results. The errors for T_k are highest for a given time; however, the ordering of the errors for the other two sensitivity coefficients are not consistent as time increases. Although not shown, the error in temperature rise will be the same as the error in the heat flux sensitivity. The line labeled "2nd order" is a reference line indicating a slope of -2; the algorithm used to numerically solve the equations is theoretically second order accurate for a spatially uniform mesh. These results confirm the approximate second order behavior of the numerical algorithm for sensitivity

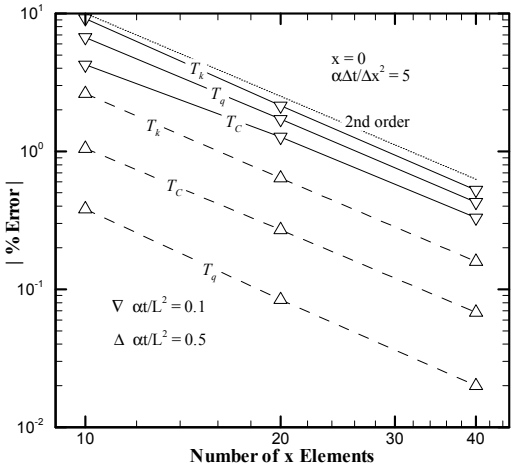


Figure 7. Grid refinement error in sensitivity coefficient calculation for 1-D planar slab with constant flux.

coefficients. The results of Fig. 7 also point out that if a certain level of accuracy is required for all sensitivity coefficients, then a different mesh may be required for each sensitivity coefficient. For example, if an error of approximately 0.4% is required, then 10, 20, and 40 elements would be required for T_q, T_C and T_k respectively for $\alpha t/L^2 = 0.5$.

Additional details on the sensitivity equation method can be found in references [12]-[30].

COMPARISON OF SEM AND DISCRETE ADJOINT METHODS FOR STEADY STATE PROBLEMS

The discrete form of the steady state energy equation can be written in matrix-vector form as

$$[K]\{T\} = \{S\} \tag{43}$$

where $[K]$ is the global conduction matrix, $\{T\}$ is the vector of unknown temperatures and $\{S\}$ is the source/right hand side vector. Sensitivity coefficients can be computed by differentiating the discrete energy equation with respect to p_i, an arbitrary element of the parameter vector $\{p\}$, to obtain

$$[K]\frac{\partial\{T\}}{\partial p_i} + \frac{\partial[K]}{\partial p_i}\{T\} = \frac{\partial\{S\}}{\partial p_i}, \quad i = 1, \ldots, n_p. \tag{44}$$

Experience indicates that scaled sensitivity coefficients, which are defined by

$$T_{p_i} = p_i \frac{\partial T}{\partial p_i} \tag{45}$$

are useful concepts. Multiplying Eq. (44) by the

nominal parameter value p_i and rearranging, the linear system of equations that determines the scaled sensitivity coefficient becomes

$$[K]\{T_{p_i}\} = p_i\frac{\partial\{S\}}{\partial p_i} - p_i\frac{\partial[K]}{\partial p_i}\{T\},\ i = 1, \ldots, n_p \quad (46)$$

For each parameter value p_i, an additional system of linear equations must be solved. This solution will give the scaled sensitivity coefficient at each nodal point in the computational domain. For parameter sensitivity studies, it may be desirable to have the sensitivity coefficient at every point in the computational domain. However, in parameter estimation work, the sensitivity coefficients may be desired only at selected locations. For example, in the estimation of thermal properties from temperature measurements, a finite number of sensors are used and the sensitivity coefficients are desired only at the temperature sensor locations.

Adjoint methods offer some potential computational savings when the number of sensor locations are few and the number of parameters are large. Following Kirsch [31], the adjoint method can be developed by multiplying the sensitivity coefficient equation, Eq. (46), by the inverse of the global conduction matrix.

$$[K]^{-1}[K]\{T_{p_i}\} = [K]^{-1}\left[p_i\frac{\partial\{S\}}{\partial p_i} - p_i\frac{\partial[K]}{\partial p_i}\{T\}\right]. \quad (47)$$

The left hand side of Eq. (47) yields the vector of sensitivity coefficients for parameter p_i at all nodal locations; however, we are only concerned with the sensitivity coefficient at a few selected locations in the computational domain. To extract the sensitivity coefficient at a single location in the computational domain, define a row-vector that has zeros everywhere except for unity at the j-th nodal location

$$\{I_j\}^T = \{0, \ldots, 0, 1, 0, \ldots 0\} \quad (48)$$

and multiply Eq. (47) by this vector results in

$$\{T_{p_i}\}_j = \{I_j\}^T[K]^{-1}[K]\{T_{p_i}\} = \{I_j\}^T[K]^{-1}\left[p_i\frac{\partial\{S\}}{\partial p_i} - p_i\frac{\partial[K]}{\partial p_i}\{T\}\right]. \quad (49)$$

Eq. (49) gives the sensitivity coefficient for parameter p_i at nodal location j. It is computationally convenient to define the coefficient of the square brackets on the right hand side of Eq. (49) as the adjoint variable vector and is

$$\{\xi_j\}^T = \{I_j\}^T[K]^{-1}. \quad (50)$$

Taking the transpose of Eq. (50) yields

$$\{\xi_j\} = ([K]^{-1})^T\{I_j\} = ([K]^T)^{-1}\{I_j\} \quad (51)$$

which can be written as

$$[K]^T\{\xi_j\} = \{I_j\},\ j = 1, \ldots, n_s. \quad (52)$$

Although Eq. (52) is valid at all n-nodal locations, the adjoint variable approach is attractive only when the number of sensors n_s is a small subset of n. Note that Eq. (52) is independent of the particular sensitivity coefficient one is trying to compute; this means that the adjoint variable vector depends only on the spatial (sensor) location in the computational domain (and $[K]$). Once Eq. (52) has been solved for the adjoint variable vector $\{\xi_j\}$, the sensitivity coefficient for all parameters of interest (at this nodal location) can be computed from Eq. (49), which is written as

$$\{T_{p_i}\}_j = \{\xi_j\}^T\left[p_i\frac{\partial\{S\}}{\partial p_i} - p_i\frac{\partial[K]}{\partial p_i}\{T\}\right],\ i = 1, \ldots, n_p. \quad (53)$$

Eq. (46) defines the discrete form of the SEM while the Eq. (52) and Eq. (53) define the discrete adjoint equations. Both approaches have a single left hand side matrix but multiple right hand side vectors. The number of right hand side vectors can be used as a rule of thumb for when one method is computationally more efficient than the other.

use SEM when $n_p < n_s$

use adjoint when $n_s < n_p$

Obviously, when n_p and n_s are approximately equal, this rule of thumb will have to be inspected more closely.

FIRST ORDER PROPAGATION OF UNCERTAINTY IN COMPUTATIONAL MODELS

Sensitivity coefficients are used in the propagation of uncertainty through computational models. The process is very analogous to experimental uncertainty estimation. Following Coleman and Steele [32], the first order uncertainty propagation equation is

$$\sigma_T^2 = \left(T_{\beta_1}\frac{\sigma_{\beta_1}}{\beta_1}\right)^2 + \left(T_{\beta_2}\frac{\sigma_{\beta_2}}{\beta_2}\right)^2 + \ldots. \quad (54)$$

Note that the uncertainty propagation equation has been written in terms of scaled sensitivity coefficients. If the sensitivity coefficients are computed at every nodal location in a

computational domain, then the uncertainty estimation due to parameter uncertainty is just a post processing of all the field variables. An uncertainty estimation for a thermally activated battery is given in Blackwell, et al. [15]. Additional details on uncertainty propagation are contained in Fadale [33] and Fadale and Emery [34].

SUMMARY

Six methods for computing sensitivity coefficients have been discussed. Example calculations were presented for several of them. The methods discussed can be divided into two broad categories; code invasive and code non-invasive. The *finite difference method* is non-invasive and probably the most general; it can be applied when the source code is not available. This means it can be used in conjunction with commercially available software. An objection to the *finite difference method* is that for non-linear problems such as temperature dependent properties, each perturbed parameter solution is a non-linear solve. If the same problem is solved using the *sensitivity equation method* (very code invasive), the sensitivity coefficient equations are linear equations. If the source code is available and the sensitivity equation method is not a viable option, then the *complex step method* should be seriously considered since it eliminates the step size issue. No matter which method is chosen to be the primary method, differentiation of analytical solutions is an important part of the process of verifying that your equations have been implemented correctly.

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