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This paper presents a general formulation of the continuous sensitivity equation method for computing first order sensitivities for transient non-linear heat conduction problems. The development of general differential equations for the sensitivities is presented for the fully non-linear heat equation. Boundary conditions are developed for both shape and value parameters. For shape parameters, this requires the extraction of first and second derivatives of the temperature along solid surfaces, a very challenging problem. The temperature and sensitivity equations are solved by a finite element method. Grid and time-step refinement studies are used to control accuracy. The proposed methodology is verified on a problem with a closed form solution using the method of manufactured solutions. The verified code is then applied to identify physical properties from a single point measurement. We demonstrate the use of sensitivities for fast computation of nearby solutions. We also use sensitivity information for cascading input data uncertainty through the finite element solver to produce uncertainty estimate of the thermal response of the system.

INTRODUCTION

Sensitivity variables are used in a wide range of engineering problems.[1] Applications include optimal design, parameter estimation, uncertainty analysis,[2] computing rate derivatives,[3] and sensitivity studies of engineering systems.[1,2]

Basically, a sensitivity is the derivative of a dependent variable with respect to a design parameter. As an example, $\frac{\partial T}{\partial k}$ is the sensitivity of the temperature with respect to k, the thermal conductivity. It expresses how the temperature field responds to perturbations of k around its nominal value. Sensitivities can also be used for fast computation of solutions at nearby values of the parameters without resorting to a full blown reanalysis or to cascade input data uncertainty through a finite element code to yield uncertainty estimates of the thermal response. Speed and cost-effectiveness are achieved by using temperature sensitivities in a Taylor expansion in the parameter space.

Dowding *et al.*[4] and Blackwell *et al.*[5] have presented sensitivity equations for conduction problems. Their work is restricted to value sensitivities and does not cover shape sensitivities. Their development is performed on the integral form used in the finite volume method. While efficient and elegant for value sensitivities, their approach leads to complications when trying to apply this for shape sensitivities, due to the delicate evaluation of mesh sensitivities. Although there are many approaches for computing sensitivity variables,[6] we emphasize the continuous sensitivity equation (CSE) approach, where the partial derivative of temperature with respect to the parameter is approximated.

This paper presents a continuous sensitivity equation method for transient non-linear heat conduction

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problems. The development is performed for value and shape sensitivities and the resulting equations are solved by a finite element method specifically designed to handle their numerical approximation.

This paper is organized as follows. First, the transient non-linear heat conduction model and boundary conditions are presented. The corresponding first order general sensitivity equations are then developed for both shape and value parameters. Some details about the numerical algorithm and the adaptative methodology follow. Next, the methodology is verified on a problem with a closed form solution and finally applied to identify physical properties from a single point measurement. Sensitivity information is also used to obtain fast computation of nearby solutions and to perform uncertainty analysis of the thermal response. The paper ends with conclusions.

NON-LINEAR HEAT CONDUCTION EQUATION

Temperature Equations

We consider the fully non-linear heat equation:

$$\rho c_p \frac{\partial T}{\partial t} = \nabla \cdot \Big(k(T) \nabla \cdot T \Big) + q \qquad (1)$$

subject to the following initial and boundary conditions:

$$\begin{aligned} T(\mathbf{x},t) &= T_b(\mathbf{x},t) \text{ on } \Gamma_D && (2)\\ -k\nabla T \cdot \mathbf{n} &= q_a(\mathbf{x},t) \text{ on } \Gamma_N && (3)\\ T(\mathbf{x},t=0) &= T_0(\mathbf{x}) && (4) \end{aligned}$$

Sensitivity Equations

The continuous sensitivity equations (CSE) are derived formally by implicit differentiation of the heat conduction equations (1)-(4), with respect to the parameter p. Thus, we treat the variable T not only as a function of space and time, but also as a function of the parameter a. This dependence is denoted as $\mathbf{T}(\mathbf{x};\mathbf{a})$. Defining the partial derivatives $s_T^a = \frac{\partial T}{\partial a}$ and the derivatives of the other variables by a (') (for example $\rho' = \frac{\partial \rho}{\partial a}$), we obtain:

$$\begin{aligned} &\rho' c_p \frac{\partial T}{\partial t} + \rho c_p' \frac{\partial T}{\partial t} + \rho c_p \frac{\partial S_T^a}{\partial t} = \\ &\nabla \cdot \Big(k'(T) \nabla \cdot T \Big) + \nabla \cdot \Big(k(T) \nabla \cdot S_T^a \Big) + q' \qquad (5) \end{aligned}$$

and the initial condition:

$$S_T^a(\mathbf{x}, t=0) = \frac{\partial T_0}{\partial a}(\mathbf{x}) \qquad (6)$$

The key point here is that we adopt a *general* approach: we consider *any* parameter a. Consequently, all of the quantities involved (temperature, material properties, coefficients, ...) may simultaneously depend on a. Therefore, all possible terms are actually included in the formulation. If any material properties are variable, then their differentiation must account for the total functional dependence.

Boundary conditions for sensitivities are also derived by implicit differentiation of equations (2)-(3). Generally speaking, the boundary can be parameter-dependent and the calculation of the sensitivities requires the extraction of the first and second order derivatives of the temperature along the solid surface. For value parameters, boundary conditions can be written:

$$S_T^a(\mathbf{x},t) = \frac{\partial T_b}{\partial a}(\mathbf{x},t) \text{ on } \Gamma_D \qquad (7)$$

$$-k'\nabla T \cdot \mathbf{n} - k \nabla S_T^a \cdot \mathbf{n} = \frac{\partial q}{\partial a}(\mathbf{x},t) \text{ on } \Gamma_N \qquad (8)$$

For shape parameters, the boundary conditions become:

$$S_T^a(\mathbf{x},t) = \frac{\partial T_b}{\partial a}(\mathbf{x},t) - \nabla T \cdot \nabla_a \mathbf{x} \text{ on } \Gamma_D \qquad (9)$$

$$\begin{aligned} -k'\nabla T \cdot \mathbf{n} - k\nabla S_T \cdot \mathbf{n} &= \frac{\partial q}{\partial a}(\mathbf{x},t) \\ &+ k\nabla\big(\nabla T \cdot \nabla_a \mathbf{x}\big) \text{ on } \Gamma_N \qquad (10) \end{aligned}$$

where

$$\nabla_a \mathbf{x} = \left(\frac{\partial x}{\partial a}, \frac{\partial y}{\partial a} \right) \qquad (11)$$

IMPLEMENTATION

The CSE has the same linearization and boundary condition types as the heat conduction equations. Therefore, the software will use a similar structure in approximating the CSE as described in.[7] The temperature and continuity equations are solved with a Galerkin finite element method.[8] The temperature is discretized using the six-nodes triangular element which uses a quadratic polynomial approximation. The adaptative remeshing procedure is modeled after that of Peraire and al.[9] and is described in more detail by Ilinca and Pelletier.[10] The procedure clusters grid points in region of rapid variation of the dependent variables. Error estimates are obtained for temperature and its sensitivities by a local least squares reconstruction of the solution derivatives.[11] For transient cases, a fixed mesh with no adaptation is used.

NUMERICAL RESULTS

Verification Problem

Our method is tested on a steady nonlinear heat conduction problem and a transient heat conduction problem.

Firstly, we test our method on the nonlinear heat conduction problem in a one-dimensional slab of thickness l assuming that the thermal conductivity is a piecewise linear function of temperature. This is the same verification problem used by Dowding *et al.*[12]

$$\frac{d}{dx}\left(k(T) \frac{dT}{dx} \right) = 0 \qquad (12)$$

$$T(0) = T_L \qquad (13)$$

$$T(l) = T_R \qquad (14)$$

where

$$k(T) = \left\{ \begin{array}{ll} k_1 \frac{T_2 - T}{T_2 - T_1} + k_2 \frac{T - T_1}{T_2 - T_1}, & T_1 \leq T \leq T_2 \\ k_2 \frac{T_3 - T}{T_3 - T_2} + k_3 \frac{T - T_2}{T_3 - T_2}, & T_2 \leq T \leq T_3 \end{array} \right\}$$

An analytical solution of this problem is presented in.[12] Expressions for the sensitivity to k_1, k_2 and k_3 are obtained by differentiating the temperature solution with respect to these parameters.

We choose to make our computations with non-dimensional variables. The domain has unit thickness, $l = 1$. The boundary temperatures are $T_L = 0$ and $T_R = 1$. Thermal conductivity is represented by two linear segments interpolating between the values k_1, k_2, and k_3 given in Table 1.

Temperature, T	0	0.5	1
Conductivity, k	1	2	6

Table 1 Conductivity definition

In Figure 1, we present the true errors in the derivatives of T as the meshes are adapted. We can easily see the second order convergence of the temperature and its sensitivities. Notice that in order to obtain

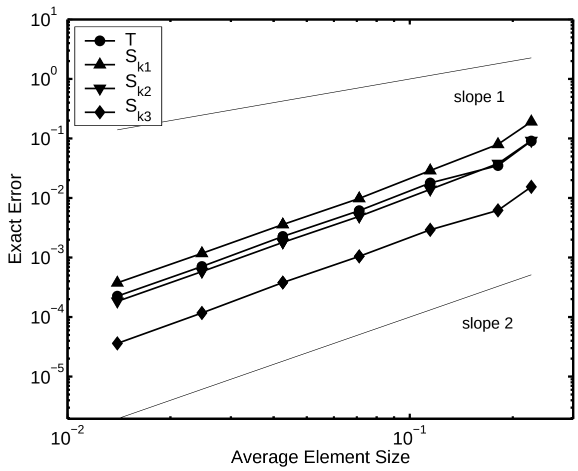

Fig. 1 Trajectories of temperature and sensitivity errors on a mesh matching conductivity interface

a convergence rate of two for the sensitivities it was necessary to divide the computational domain in two zones, the interface between the zones coinciding with the line of discontinuity of the derivative of the piecewise linear conductivity k. For a general mesh, as mentioned in,[12] the sensitivities achieve only first order accuracy (see Figure 2).

Next, we want to verify our method on the non-linear transient heat conduction equation using manufactured[13] and exact solutions[14] and we will perform a systematic grid and time-step refinement studies to verify the convergence rate of the finite element solutions of heat conduction equation and its sensitivity equations.

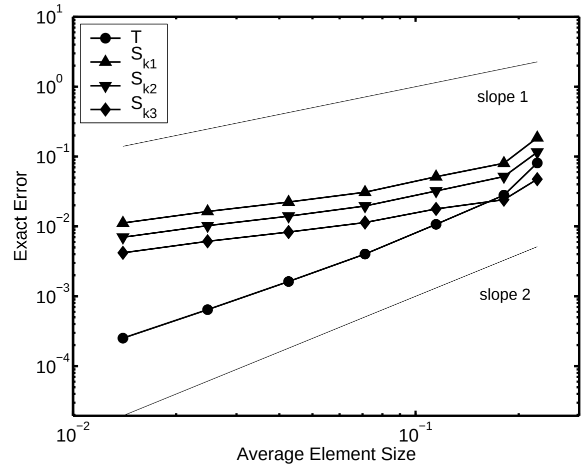

Fig. 2 Grid convergence on a mesh not matching conductivity interface.

We have constructed a one-dimension non-linear transient analytical solution in a two-dimension domain.

$$\begin{aligned} T(x,t) &= e^{-A(x-x_0)^2} \qquad (15) \\ x_0 &= Rsin(2\pi t) + x_c \\ \Omega &= [0,1] \times [0,0.2], t \in [0,0.25] \end{aligned}$$

The following non-dimensional physical properties are constants: $\rho = 1$, $c_p = 1$. The thermal conductivity is a linear function of temperature for which the values of k_1 and k_2 with their corresponding temperatures are given in Table 2.

$$k(T) = k_1 \left(\frac{T_2 - T}{T_2 - T_1} \right) + k_2 \left(\frac{T - T_1}{T_2 - T_1} \right) \qquad (16)$$

where

Temperature, T	0	1
Conductivity, k	0.5	1

Table 2 Conductivity definition

The values of parameters which describe the temperature definition are:

$$A = 10, R = 0.3, x_c = 0.5$$

where R and A are the sensitivity parameters.

To satisfy the non-linear transient heat conduction, we add a source term in the solved equation calculated as follow:

$$q(x,t) = \rho cp \frac{\delta T}{\delta t} - \nabla (k \nabla T) \qquad (17)$$

Any combinations of Dirichlet and Neumann boundary conditions type can be applied on the domain. We choose to apply Dirichlet condition on boundaries which takes the value of the analytical solution evaluted at the boundary. The analytical solution evaluated at initial time $t = 0$ is applied as initial condition.

A time-step and grid convergence study for the temperature and its sensitivity is shown in Figure 3. To demonstrate this double convegence (time-step and grid), we have performed simulations described in Table 3. The temperature, as well as its sensitivity, demonstrates a fourth-order accuracy with the refinement of the time steps and grid.

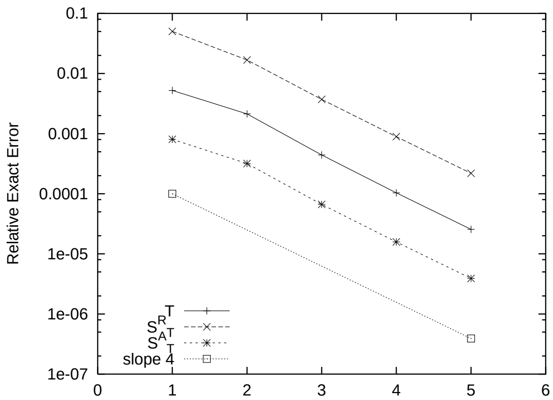

Fig. 3 Time and grid convergence of temperature and its sensitivities

	Mesh		Crank-Nicholson	
	N_{el}	h	$N_{\Delta t}$	Δt
1	50	0.131277	5	0.05
2	200	0.064958	10	0.025
3	800	0.032904	20	0.0125
4	3200	0.015749	40	0.00625
5	12810	0.007833	80	0.003125

Table 3 Grid and time steps definition

We use a second-order integration scheme (Cank-Nicholson) for the transient computation, thus we have a second-order solver in space and time. For each simulation we divide by two time-step and elements size which means to divide exact error by four.

These results confirm the correctness of the implementation of the first order sensitivities in the solver and verify the calculation of the continuous first order sensitivity equations by the adaptative finite element solver.

Transient non-linear problem

We consider an experimental design for estimating linearly varying temperature-dependent properties from a single experiment. The configuration was proposed by Dowding *et al.*[12] for polyurethane foam. Two identical specimen of foam of thickness L_f, separated by a heater of thickness $2L_h$, are sandwiched between two aluminum blocks. The cross-section of all components is the same. A two dimensional model of the experiment is showed on Figure 4. Because of the symmetry of the problem only one half of the configuration is presented. Also, as the role of the aluminum block is to maintain a constant temperature on the wall opposite to the heater, it was replaced in our model by an isothermal boundary condition. All other walls are considered adiabatic. By knowing the input heat flux and measuring the temperature elsewhere in the domain, the thermal properties of the foam can be estimated. Dowding *et al.*[12] compare two different configurations where the foam react as a finite or a semi-infinite body. They show using the D-optimality criterium that the finite body is better for estimating the thermal properties of the foam. In our calculations we will consider only the finite body configuration.

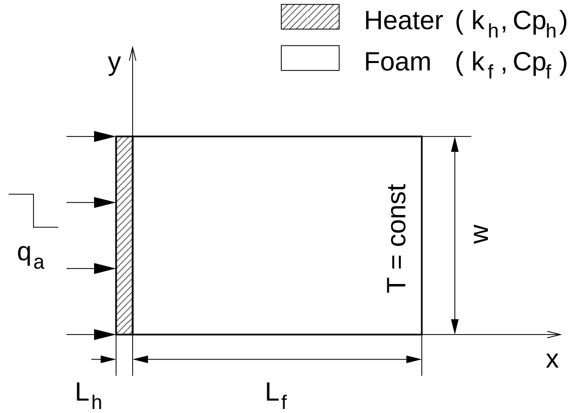

Fig. 4 Two dimensional model of an experiment to estimate thermal properties of polyurethane foam.

The values of the different parameters of the problem are given in Table 4. The thermal properties of the heater, conductivity and volumetric heat capacity ($C = \rho C_p$), are constant. Those of the foam are linearly dependent on the temperature.

$$k_f(T) = \kappa\Big(k_1\frac{T_2 - T}{T_2 - T_1} + k_2\frac{T - T_1}{T_2 - T_1}\Big) \quad (18)$$

$$C_f(T) = \gamma\Big(C_1\frac{T_2 - T}{T_2 - T_1} + C_2\frac{T - T_1}{T_2 - T_1}\Big) \quad (19)$$

The parameters κ and γ are introduced for convenience in the sensitivity analysis. They are set to one. The sensitivity to these parameters will allow us later to produce uncertainty estimate of the thermal response of the system. Simulated temperature response for a foam thickness of 2.54 cm is shown in figure 5. Two measurement locations are simulated: one at the heated surface ($x = 0$) and the other in the middle of the foam layer ($x = 0.5$). The imposed heat flux ends at $t = 1.5 \times 10^4 s$ corresponding the dimensionless $\tilde{t} = 2.68$ on the different figures. The scaled sensitivity coefficients ($\frac{a_0 S^a_T}{T_{max}}$) for the four parameters k_1, k_2, C_1, C_2 and the two mesurement locations are shown in Figures 6 and 7. Theses coefficients are normalized by the maximum temperature rise. The results presented are as accurate as those obtained by Dowding[12] with a finite volume method. In our simulation, we include the sensitivities with respect to κ and γ, which provide an additional information on the linearly dependent

	dimensional	non-dimensional
L_h	$0.63\,mm$	0.0248
k_h	$0.1\,W/mK$	2.0
C_h	$2.3E+06\,J/m^3K$	5.31178
L_f	$2.54\,cm$	1.0
k_1	$0.05\,W/mK$	1.0
k_2	$0.102\,W/mK$	2.04
C_1	$0.433E+06\,J/m^3K$	1.0
C_2	$1.19E+06\,J/m^3K$	2.74827
T_1	$25\,°C$	0.125
T_2	$200\,°C$	1.0
q_a	$500\,W/m^2$	1.27

Table 4 Parameter definition

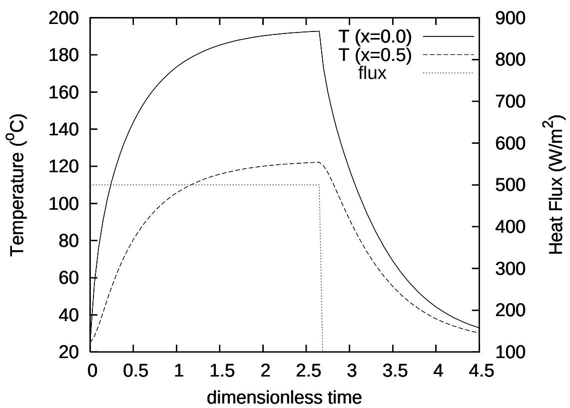

Fig. 5 Temperature response for a foam thickness of 2.54 cm with linearly varying temperature dependent properties.

properties. Furthermore, we also solve the sensitivity equation for the shape parameter L_f (thickness of the foam). The results are plotted in Figure 8 and 9. Notice how the shapes of the sensitivity coefficients change when the heat flux ends, especially for C_1, C_2, and γ, which actually change signs. In addition, the sensitivity coefficient for L_f is larger than the other coefficients. In the design of experiments, large and uncorrelated scaled sensitivities lead to better estimates of the thermal response. We follow here the steps of Dowding *et al.* by providing a sensitivity analysis in order to determine the optimum experimental configuration to estimate the temperature-dependent variables. In most cases, a known input heat flux permits conductivity and volumetric heat capacity to be simultaneously estimated from a single experiment by applying a sequential method (Beck and Osman[15]).

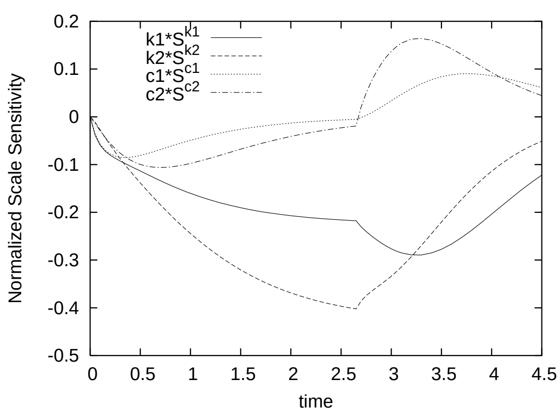

Fig. 6 Sensitivities normalized by the maximum temperature rise at $x = 0$

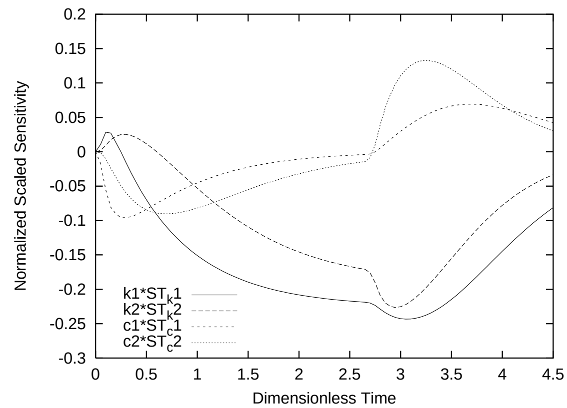

Fig. 7 Sensitivities normalized by the maximum temperature rise at $x = 5$

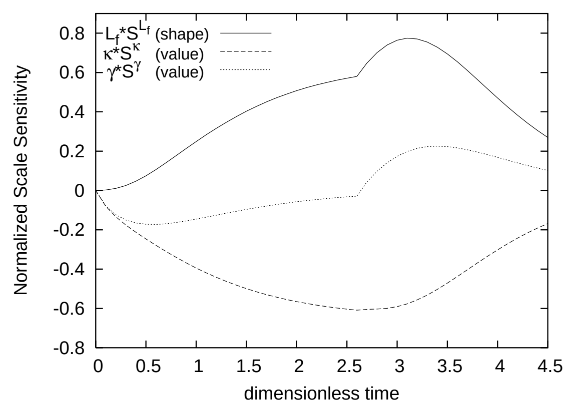

Fig. 8 Sensitivities normalized by the maximum temperature rise at $x = 0$

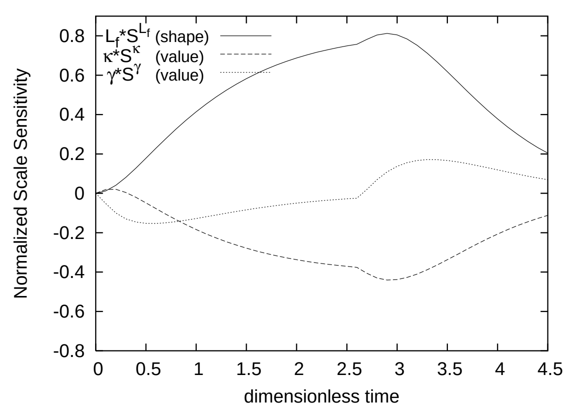

Fig. 9 Sensitivities normalized by the maximum temperature rise at $x = 0.5$

The use of sensitivity coefficients for fast computation of nearby solutions is demonstrated in Figure 10 for the shape parameter L_f. The exact and estimated temperature are plotted for a variation of 10% of the foam thickness and the results show an accurate linear extrapolation. In a physical experiment, we recognize that there are both measurement uncertainties in the experimental data as well as uncertainties in the parameters. In our study, sensitivity analysis is combined with linear Taylor-like estimates to provide uncertainty bands for numerical simulations. These can then be compared to experimental measurements. If we group our parameters in the vector $\mathbf{a} = (a_1, ..., a_n)$, then if $\mathbf{a}$ is perturbed by $\Delta\mathbf{a}$, the temperature variation may be approximated as follows:

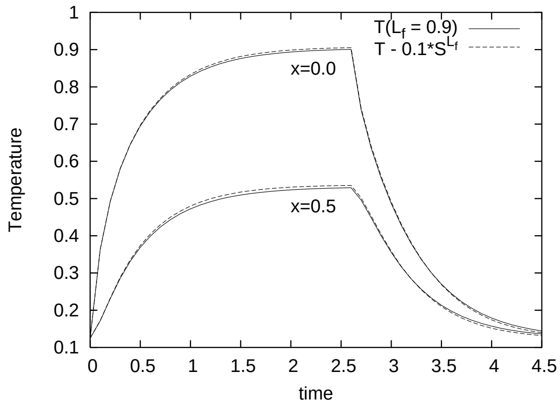

Fig. 10 Exact and Extrapolated thermal response for $\frac{\Delta L_f}{L_f} = 10\%$

$$|T(x; \mathbf{a} + \Delta\mathbf{a}) - T(x; \mathbf{a})| \leq \sum_{i=1}^{n} \left| \frac{\partial T}{\partial a_i}(x; \mathbf{a}) \Delta a_i \right| \quad (20)$$

We present in Figure 11 the contributions to the uncertainty calculations from the parameters κ and γ. Here we use the following uncertainty bounds: $\kappa \pm 0.1$ and $\gamma \pm 0.1$. Note the tighter bound at $x = 0.5$.

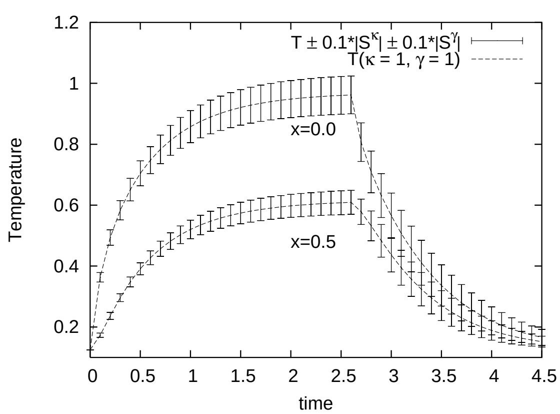

Fig. 11 Temperature at $x = 0$ and $x = 0.5$ with Uncertainty Bands

CONCLUSION

A general formulation of the continuous sensitivity equation for transient nonlinear heat conduction problems was computed through an finite element code and tested on a problem with a closed form solution. The verified code was then applied to identify linearly varying temperature-dependent properties in a finite polyurethane foam. Parametric sensitivity analysis allowed us to find the influence of both value and shape parameters on the state of the system. We then demonstrated the use of the sensitivity coefficients for fast computation of nearby solutions. Sensitivity information was also computed to produce uncertainty estimates of the thermal response.

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