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**A 3-D FINITE ELEMENT FORMULATION FOR THE DETERMINATION OF
UNKNOWN BOUNDARY CONDITIONS IN HEAT CONDUCTION**

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ABSTRACT

A 3-D finite element method (FEM) formulation for the detection of unknown steady boundary conditions in heat conduction is presented. The present FEM formulation is capable of determining temperatures and heat fluxes on the boundaries where such quantities are unknown or inaccessible, provided such quantities are sufficiently over-specified on other boundaries. A regularized form of the method is also presented. The regularization is necessary for solving problems where the over-specified boundary data contains errors. Details of the discretization and regularization and sample results for a 3-D problem are presented.

KEYWORDS

inverse problems, finite element method, inverse heat conduction

NOMENCLATURE

$[D]$	Damping matrix
$[K_c]$	Stiffness matrix
k	Fourier coefficient of heat conduction
Q	Heat flux vector
\bar{q}	Heat flux
R	Uniform random number between 0 and 1
S	Heat source
v	Weighting function
x, y, z	Cartesian body axes
Γ	Boundary surface
Λ	Damping parameter

σ	Standard deviation
Θ	Temperature

INTRODUCTION

It is often difficult or even impossible to place temperature probes, heat flux probes, or strain gauges on certain parts of a surface of a solid body. This can be due to its small size, geometric inaccessibility, or a exposure to a hostile environment. With an appropriate inverse method these unknown boundary values can be determined from additional information provided at the boundaries where the values can be measured directly. In the case of steady thermal and elastic problems, the objective of the inverse problem is to determine displacements, surface stresses, heat fluxes, and temperatures on boundaries where they are unknown. The problem of inverse determination of unknown boundary conditions in two-dimensional steady heat conduction has been solved by a variety of methods [1, 2, 3, 4, 5]. Similarly, a separate inverse boundary condition determination problem in linear elastostatics has been solved by different methods [6]. The inverse boundary condition determination problem for steady thermoelasticity was also solved for several two-dimensional problems [4].

A 3-D finite element formulation is presented here that allows one to solve this inverse problem in a direct manner by over-specifying boundary conditions on boundaries where that information is available. Our objective is to develop and demonstrate an approach for the prediction of thermal boundary conditions on parts of a three-dimensional solid body surface by using FEM.

It should be pointed out that the method for the solution of inverse problems to be discussed in this paper is different from the approach based on boundary element method that has been used separately in linear heat conduction [3] and linear elasticity [6].

For inverse problems, the unknown boundary conditions on parts of the boundary can be determined by overspecifying the boundary conditions (enforcing both Dirichlet and Neumann type boundary conditions) on at least some of the remaining portions of the boundary, and providing either Dirichlet or Neumann type boundary conditions on the rest of the boundary. It is possible, after a series of algebraic manipulations, to transform the original system of equations into a system which enforces the overspecified boundary conditions and includes the unknown boundary conditions as a part of the unknown solution vector. This formulation is an adaptation of a method used by Martin and Dulikravich [7] for the inverse detection of boundary conditions in steady heat conduction.

Specifically, this work represents an extension of the conceptual work presented by the authors [4] by extending the original formulation from two dimensions into three dimensions.

FEM FORMULATION FOR HEAT CONDUCTION

The temperature distribution throughout the solid domain can be found by solving Poisson's equation for steady linear heat conduction with a distributed steady heat source function, S , and

thermal conductivity coefficient, k ,

$$-k\left(\frac{\partial^2 \Theta}{\partial x^2} + \frac{\partial^2 \Theta}{\partial y^2} + \frac{\partial^2 \Theta}{\partial z^2}\right) = S \quad (1)$$

Applying the method of weighted residuals to (1) over an element results in

$$\int_{\Omega^e} \left(\frac{\partial^2 \Theta}{\partial x^2} + \frac{\partial^2 \Theta}{\partial y^2} + \frac{\partial^2 \Theta}{\partial z^2} - \frac{S}{k}\right)v \, d\Omega^e = 0 \quad (2)$$

Integrating this by parts once (2) creates the weak statement for an element

$$\begin{aligned} & - \int_{\Omega^e} k \left(\frac{\partial v}{\partial x} \frac{\partial \Theta}{\partial x} + \frac{\partial v}{\partial y} \frac{\partial \Theta}{\partial y} + \frac{\partial v}{\partial z} \frac{\partial \Theta}{\partial z} \right) d\Omega^e \\ & = \int_{\Omega^e} N_i S \, d\Omega^e - \int_{\Gamma^e} N_i (\vec{q} \cdot \hat{n}) \, d\Omega^e \end{aligned} \quad (3)$$

Variation of the temperature across an element can be expressed by

$$\Theta(x, y, z) \approx \tilde{\Theta}^e(x, y, z) = \sum_{i=1}^m N_i(x, y, z) \Theta_i \quad (4)$$

Using Galerkin's method, the weight function v and the interpolation function for Θ are chosen to be the same.

By defining the matrix $[B]$ as

$$[B] = \begin{bmatrix} \frac{\partial N_1}{\partial x} & \frac{\partial N_2}{\partial x} & \dots & \frac{\partial N_m}{\partial x} \\ \frac{\partial N_1}{\partial y} & \frac{\partial N_2}{\partial y} & \dots & \frac{\partial N_m}{\partial y} \\ \frac{\partial N_1}{\partial z} & \frac{\partial N_2}{\partial z} & \dots & \frac{\partial N_m}{\partial z} \end{bmatrix} \quad (5)$$

the weak statement (3) can be written in the matrix form as

$$[K_c^e] \{\Theta^e\} = \{S^e\} \quad (6)$$

where

$$[K_c^e] = \int_{\Omega^e} k [B]^T [B] \, d\Omega^e \quad (7)$$

$$\{Q^e\} = - \int_{\Omega^e} S \{N\} \, d\Omega + \int_{\Gamma^e} q_s \{N\} \, d\Gamma^e \quad (8)$$

The local stiffness matrix, $[K_c^e]$, and heat flux vector, $\{Q^e\}$, are determined for each element in the domain and then assembled into the global system of linear algebraic equations.

$$[K_c] \{\Theta\} = \{Q\} \quad (9)$$

DIRECT AND INVERSE FORMULATIONS

The above equations for steady heat conduction were discretized by using a Galerkin's finite element method. The system is typically large, sparse, symmetric, and positive definite. Once the global system has been formed, the boundary conditions are applied. For a well-posed analysis (direct) problem, the boundary conditions must be known on all boundaries of the domain. For

heat conduction, either the temperature, Θ_s , or the heat flux, Q_s , must be specified at each point of the boundary.

For an inverse problem, the unknown boundary conditions on parts of the boundary can be determined by over-specifying the boundary conditions (enforcing both Dirichlet and Neumann type boundary conditions) on at least some of the remaining portions of the boundary, and providing either Dirichlet or Neumann type boundary conditions on the rest of the boundary. It is possible, after a series of algebraic manipulations, to transform the original system of equations into a system which enforces the over-specified boundary conditions and includes the unknown boundary conditions as a part of the unknown solution vector. As an example, consider the linear system for heat conduction on a tetrahedral finite element with boundary conditions given at nodes 1 and 4.

$$\begin{bmatrix} K_{11} & K_{12} & K_{13} & K_{14} \\ K_{21} & K_{22} & K_{23} & K_{24} \\ K_{31} & K_{32} & K_{33} & K_{34} \\ K_{41} & K_{42} & K_{43} & K_{44} \end{bmatrix} \begin{Bmatrix} \Theta_1 \\ \Theta_2 \\ \Theta_3 \\ \Theta_4 \end{Bmatrix} = \begin{Bmatrix} Q_1 \\ Q_2 \\ Q_3 \\ Q_4 \end{Bmatrix} \quad (10)$$

As an example of an inverse problem, one could specify both the temperature, Θ_s , and the heat flux, Q_s , at node 1, flux only at nodes 2 and 3, and assume the boundary conditions at node 4 as being unknown. The original system of equations (10) can be modified by adding a row and a column corresponding to the additional equation for the over-specified flux at node 1 and the additional unknown due to the unknown boundary flux at node 4. The result is

$$\begin{bmatrix} 1 & 0 & 0 & 0 & 0 \\ K_{21} & K_{22} & K_{23} & K_{24} & 0 \\ K_{31} & K_{32} & K_{33} & K_{34} & 0 \\ K_{41} & K_{42} & K_{43} & K_{44} & -1 \\ K_{11} & K_{12} & K_{13} & K_{14} & 0 \end{bmatrix} \begin{Bmatrix} \Theta_1 \\ \Theta_2 \\ \Theta_3 \\ \Theta_4 \\ Q_4 \end{Bmatrix} = \begin{Bmatrix} \Theta_s \\ Q_2 \\ Q_3 \\ 0 \\ Q_s \end{Bmatrix} \quad (11)$$

The resulting systems of equations will remain sparse, but will be non-symmetric and possibly rectangular (instead of square) depending on the ratio of the number of known to unknown boundary conditions.

REGULARIZATION

Two regularization methods were applied separately to the iterative solution of the systems of equations in attempts to increase the method's tolerance for possible measurement errors in the over-specified boundary conditions.

The general form of a regularized system is given as [8]:

$$\begin{bmatrix} K_c \\ \Lambda D \end{bmatrix} \{\Theta\} = \begin{Bmatrix} Q \\ 0 \end{Bmatrix} \quad (12)$$

The traditional Tikhonov regularization [9] is obtained when the damping matrix, $[D]$, is set equal to the identity matrix. Solving (12) in a least squares sense minimizes the following error function.

$$error(\Theta) = \|[K_c]\{\Theta\} - \{Q\}\|^2 + \|\Lambda[D]\{\Theta\}\|^2 \quad (13)$$

This is the minimization of the residual plus a penalty term. The form of the damping matrix determines what penalty is used and the damping parameter, Λ , weights the penalty for each equation. These weights should be determined according to the error associated with the respective equation.

Method 1

This method of regularization uses a constant damping parameter Λ over the entire domain and the identity matrix as the damping matrix. This method can be considered the traditional Tikhonov method. The penalty term being minimized in this case is the square of the L_2 norm of the solution vector $\{x\}$. Minimizing this norm will tend to drive the components of $\{x\}$ to uniform values thus producing a smoothing effect. However, minimizing this penalty term will ultimately drive each component to zero, completely destroying the real solution. Thus, great care must be exercised in choosing the damping parameter Λ so that a good balance of smoothness and accuracy is achieved.

Method 2

This method of regularization uses a constant damping parameter Λ only for equations corresponding to the unknown boundary values. For all other equations, $\Lambda = 0$ and $[D] = [I]$ is used since the largest errors occur at the boundaries where the temperatures and fluxes are unknown.

SOLUTION OF THE LINEAR SYSTEM

In general, the resulting FEM systems for the inverse thermal conductivity problems are sparse, unsymmetric, and often rectangular. These properties make the process of finding a solution to the system very challenging. Three approaches will be discussed here.

The first is to normalize the equations by multiplying both sides by the matrix transpose and solve the resulting square system with common sparse solvers.

$$[K]^T[K]\{\Theta\} = [K]^T\{Q\} \quad (14)$$

This approach has been found to be effective for certain inverse problems [10]. The resulting normalized system is less sparse than the original system, but it is square, symmetric, and positive definite with application of regularization. The normalized system is solved with a direct method (Cholesky or LU factorization) or with an iterative method (preconditioned Krylov subspace). There are several disadvantages to this approach. Among them being the expense of computing $[K]^T[K]$, the large in-core memory requirements, and the roundoff error incurred during the $[K]^T[K]$ multiplication.

Another approach is to use iterative methods suitable for non-symmetrical and least squares problems. One such method is the LSQR method, which is an extension of the well-known conjugate gradient method [11]. The LSQR method and other similar methods such as the conjugate gradient for least squares (CGLS) solve the normalized system, but without explicit computation of $[K]^T[K]$. However, convergence rates of these methods depend strongly on the condition number of the normalized system which is roughly the condition number of $[K]$ squared. Convergence can be slow when solving the systems resulting from the inverse finite element discretization since they are ill-conditioned.

Yet another approach is to use a non-iterative method for non-symmetrical and least squares problems such as QR factorization or SVD [12]. However, sparse implementations of QR or SVD solvers are needed to reduce the in-core memory requirements for the inverse finite element problems. It is also possible to use static condensation to reduce the complete sparse system of equations into a dense matrix of smaller dimensions [5]. The reduced system involves only the unknowns on the boundary of the domain and can be solved efficiently using standard QR or SVD algorithms for dense matrices.

NUMERICAL RESULTS

The accuracy and efficiency of the finite element inverse formulation was tested on several simple three-dimensional problems. The method was implemented in an object-oriented finite element code written in C++. Elements used in the calculations were hexahedra with tri-linear interpolation functions. The linear systems were solved with a sparse QR factorization. The basic test geometry is an annular cylinder.

The hexahedral mesh is shown in Figure 1. The outer surface has a radius of 3.0 and the inner surface has a radius of 2.0. The mesh is composed of 1440 elements and 1980 nodes. The inner and outer boundaries each have 396 nodes. For this geometry, there is an analytical solution if constant temperature boundary conditions are used on the inner and outer boundaries. In a direct (well-posed) problem a uniform temperature of 10.0 C was enforced on the inner boundary while a temperature of -10.0 C was enforced on the outer boundary. Adiabatic conditions were specified at the ends of the cylinder. The computed temperature field is shown in Figure 2. The temperature field computed with the FEM had a maximum error of 1.0% compared to the analytical solution.

The inverse problem was then created by over-specifying the outer cylindrical boundary with the double-precision values of temperatures and fluxes obtained from the analysis case. At the same time, no boundary conditions were specified on the inner cylindrical boundary [3]. A damping parameter of $\Lambda = 0$ was used. The computed temperature distribution is shown in Figure 3. The maximum relative differences in temperatures between the analysis and inverse results are less than 0.1% when solved using the QR factorization.

The above problem was repeated for boundary conditions with random measurement errors added. For these cases, regularization was used. Random errors in the known boundary temperatures and fluxes were generated using the following equations [3]:

$$\Theta = \Theta_{bc} \pm \sqrt{-2\sigma^2 \ln R} \quad (15)$$

$$Q = Q_{bc} \pm \sqrt{-2\sigma^2 \ln R} \quad (16)$$

For each case, Eqns. (15)-(16) were used to generate errors in both the known boundary fluxes and temperatures obtained from the forward solution.

First, regularization method 1 was used with a wide range of damping parameters. The average percent error of the predicted temperatures on the unknown boundaries as a function of damping parameter and various levels of measurement error is shown in Figure 4.

The inverse problem was also solved using regularization method 2 for a wide range of damping parameters. The average percent error of the predicted temperatures on the unknown boundary as a function of damping parameter is shown in Figure 5.

Results indicate that the present formulation is capable of predicting the unknown boundary conditions with errors on the same order of magnitude as the errors in the over-specified data. In other words, both regularization methods prevent the amplification of the measurement errors. Regularization method 2 achieved slightly more accurate results than method 1 for all levels of random measurement error.

The lack of error amplification with this method may only occur for simple geometries. Results in 2-D indicate that more sophisticated regularization techniques are necessary for complicated geometries such as multiply connected domains [4]. The present 3-D FEM inverse method will likely require better regularization methods if measurement errors are used with complicated multiply-connected three-dimensional geometries.

CONCLUSIONS

A formulation for the inverse determination of unknown steady boundary conditions in heat conduction for three-dimensional problems has been developed using FEM. The formulation has been tested numerically using an annular geometry with a known analytic solution. The formulation can predict the temperatures on the unknown boundary with high accuracy in the annular domain without the need for regularization. However, regularization was required in order to compute a good solution when measurement errors in the over-specified boundary conditions were added. Two different regularization methods were applied. Both allow a stable QR factorization to be computed, but neither resulted in highly accurate temperature predictions on the unknown boundaries for large values of measurement errors. However, both regularization methods prevented amplification of the measurement errors. Further research is needed to develop better regularization methods so that the present formulation can be made more robust with respect to measurement errors used with more complex geometries.

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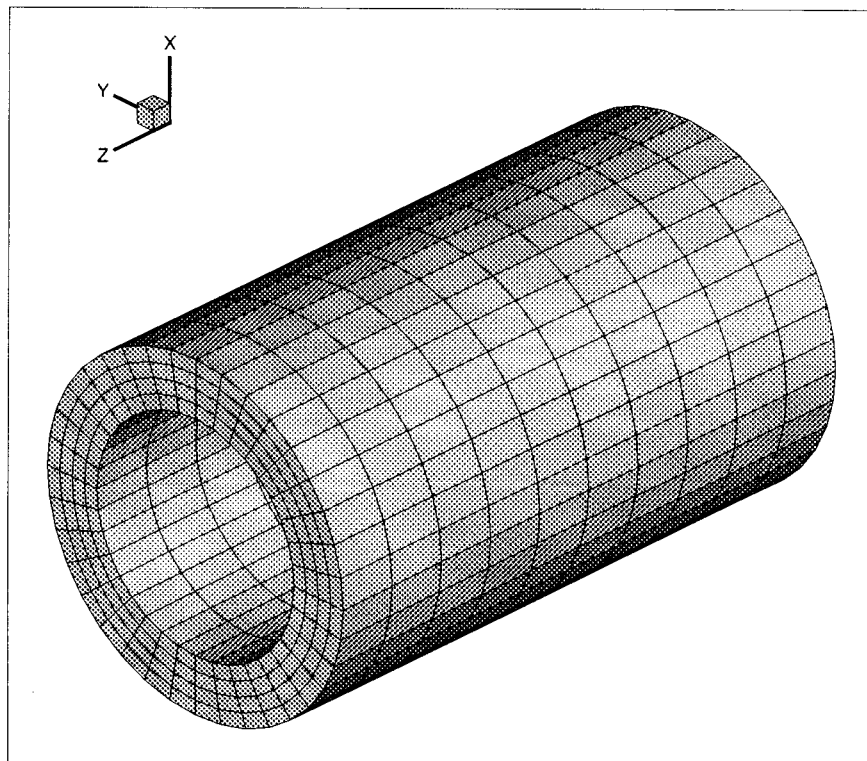


Figure 1: Hexahedral mesh for an annular cylinder test case geometry

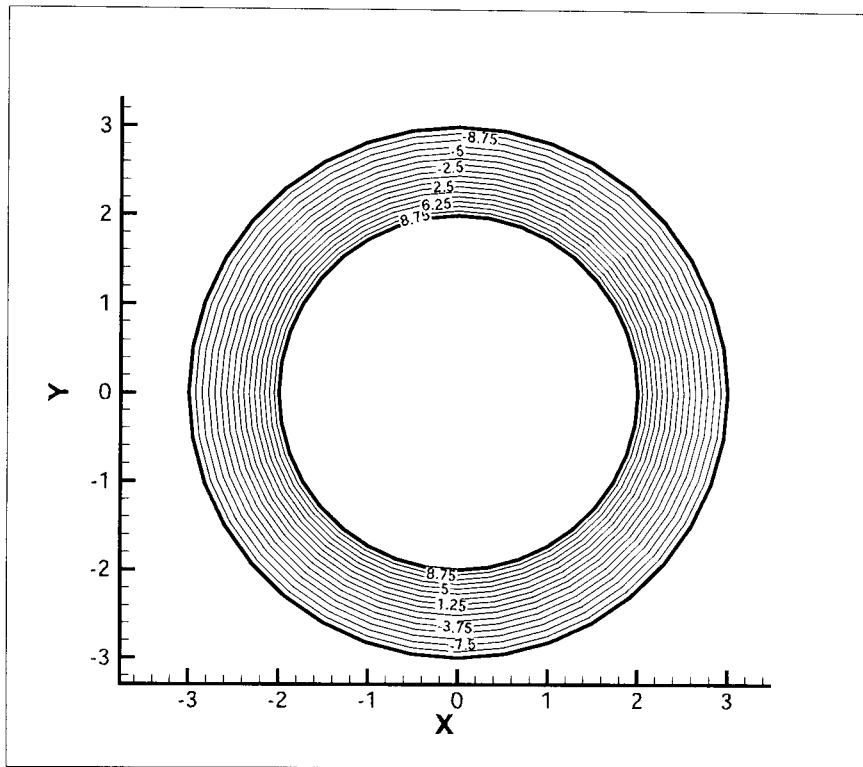


Figure 2: Direct problem: computed isotherms when both inner and outer boundary temperatures were specified

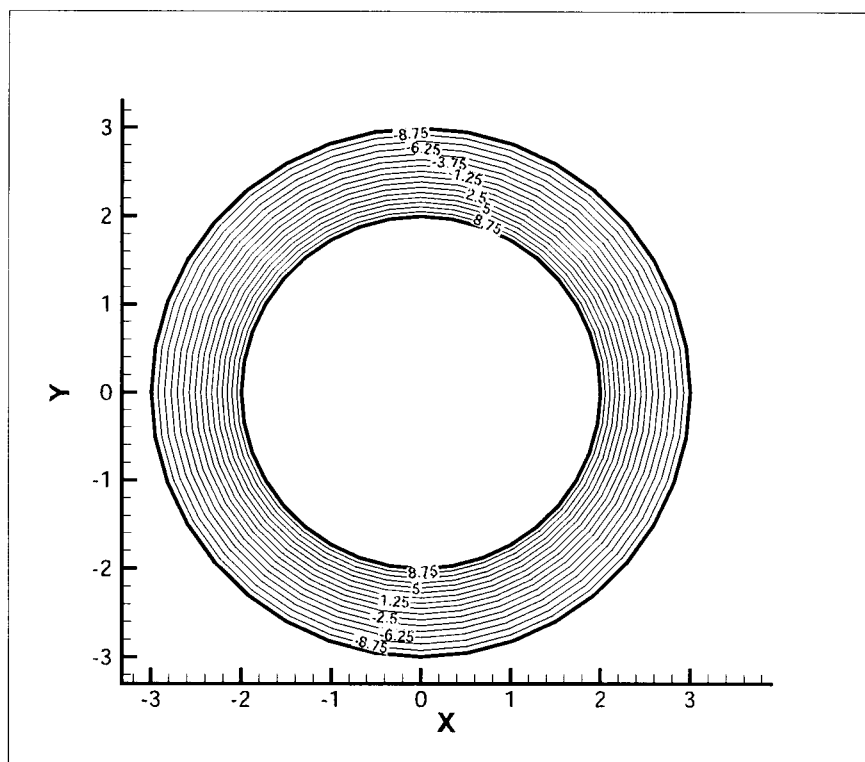


Figure 3: Inverse problem: computed isotherms when only outer boundary temperatures and fluxes were specified

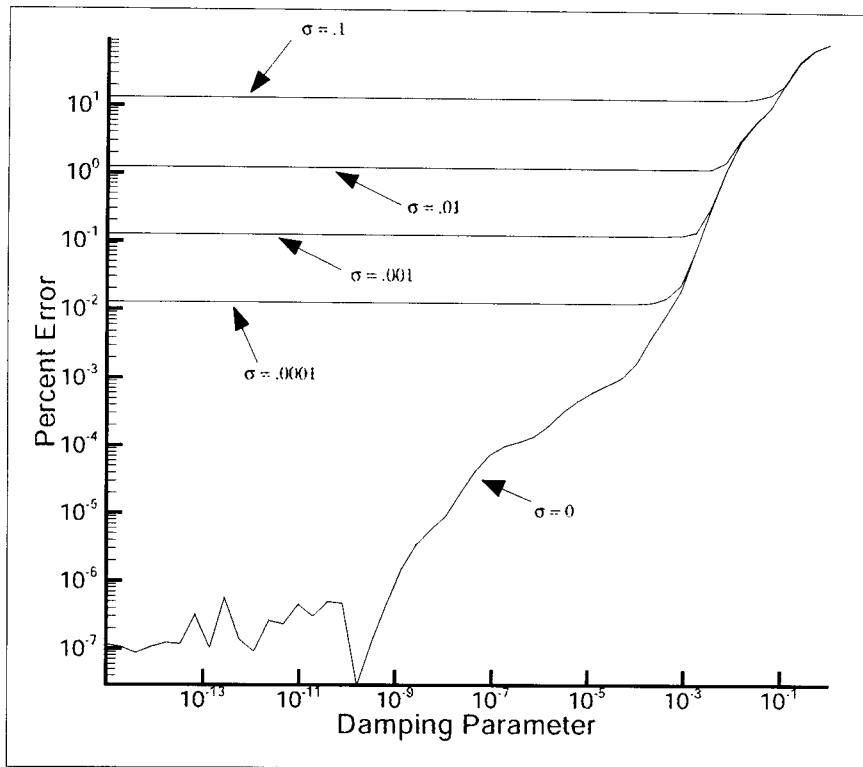


Figure 4: Computed average percent error in temperature on unknown boundaries for regularization method 1

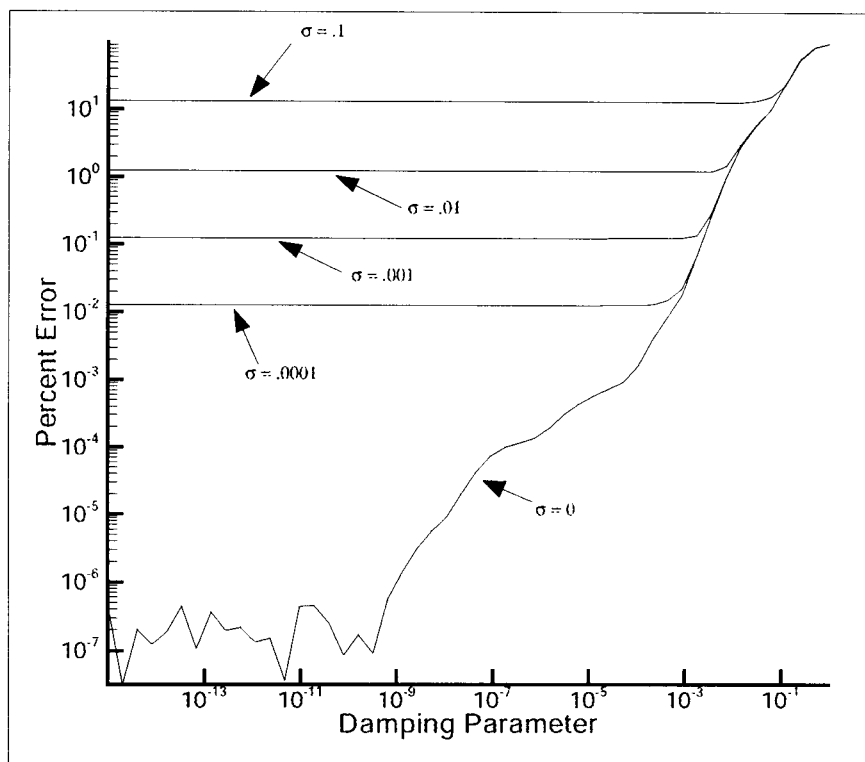


Figure 5: Computed average percent error in temperature on unknown boundaries for regularization method 2