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THE JAPAN SOCIETY OF MECHANICAL ENGINEERS
Shinanomachi Renga-kan 5 Floor, 35 Shinanomachi,
Shinjuku, Tokyo 160, Japan
Phone: 81(Japan)-3-5360-3500; Fax: 81(Japan)-3-5360-3507

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MULTIDISCIPLINARY INVERSE PROBLEMS AND SOLUTION METHODS

George S. Dulikravich[1] and Thomas J. Martin[2]
Department of Aerospace Engineering
The Pennsylvania State University
University Park, PA 16802, USA
Phone: +1-814-863-0134, Fax: +1-814-865-7092
E-mail: gsd@ecl.psu.edu or ft7@psu.edu

ABSTRACT

An inverse Boundary Element Method (BEM) procedure has been developed to determine unknown steady boundary conditions (temperatures, heat fluxes, heat convection coefficients, deformations, and stresses) on surfaces of arbitrarily shaped solids. With this technique, boundary conditions of Dirichlet or Neumann type could be measured on only certain parts of the boundary that are easily accessible. Over-specified (both Dirichlet and Neumann types) boundary conditions, or internal measurements, on other, more accessible boundaries, must be provided in order to compensate for the unknown boundary conditions. An ill-conditioned matrix resulting from this inverse BEM formulation must be properly inverted to obtain the solution to the ill-posed problem. The method is very fast because it is non-iterative. Accuracy of numerical results has been demonstrated for several steady two-dimensional heat transfer and elasticity problems. The method is very robust and not too sensitivity to errors in the measurement data.

INTRODUCTION

It is very often the case in practical engineering applications that we need to know certain field variable (temperature, heat flux, heat convection coefficient, deformations, stresses, electric potential, etc.) on boundary or surface of realistically-shaped objects that are made of components having different physical properties. These boundary conditions can be steady or time-dependent. This paper explains how to determine steady boundary conditions on surfaces where it is impossible to perform the measurement because these surfaces are either too small and inaccessible or they are exposed to an extremely hostile environment that would destroy the sensors. Thus, we will concentrate on field problems that can be modeled as steady boundary condition problems. Examples are steady temperature fields, electrostatic fields, stress/deformation fields, etc.

A well-posed (or direct, or analysis) steady boundary value problem requires either the field variables or their derivatives normal to the boundary to be known over the entire boundary of the solid object.

An ill-posed (or inverse, or design, or parameter estimation) steady boundary condition problem requires that boundary conditions are entirely unknown on some parts of the boundary. On some of the remaining parts of the boundary, either the field variables or their derivatives normal to the boundary must be known.

In order to make the inverse problems solvable, additional information must be provided either in the form of field variable measurements at a number of points inside the object or in the form of over-specified boundary conditions on the remaining parts of the boundary [1]. For example, providing an over-specified boundary condition in steady heat conduction would mean that we have to measure both surface temperature and surface heat flux at the same boundary points on at least a part of the object's boundary.

Another class of inverse problems arises when the size and shape of some parts of the domain are unknown. In order to determine the remaining geometry of the domain, we must know additional boundary conditions in the form of independently specified Dirichlet and Neumann boundary conditions at the same points of the known boundary. Thus, when the thermal boundary conditions are over-specified on a part of the boundary and the remaining boundary is not known, the problem is referred to as an inverse shape design or problem [2-5] or shape identification problem [6-7].

There are many numerical methods that are capable of solving different types of inverse boundary condition problems [8-10]. Most of the solution methods are iterative, thus requiring sophisticated regularization techniques in order to keep the numerical error from growing exponentially during the iterations [11]. Some of the solution methods utilize optimization algorithms to minimize the difference between the measured and the predicted boundary conditions. This approach is particularly unreliable because the process can converge to a local minimum [12].

We have developed a non-iterative algorithm [12, 13] that reliably and efficiently solves inverse steady boundary condition problems governed by the Laplace

[1] Associate Professor. Fellow ASME.
[2] Graduate Research Assistant. Student member ASME.

equation in two-dimensional and three-dimensional multiply-connected domains having different material properties [14-15]. Different versions of this method were used in solving inverse problems of determining heat convection coefficients [16], temperature-dependent thermal conductivities [17], boundary stresses and deformations in two-dimensional elasticity [18], as well as for the determination of heat sources [13]. This technique is based on the Green's function solution method [19, 20], commonly referred to as the Boundary Element Method (BEM). This method results in a full matrix of geometric coefficients. For well-posed problems, the matrix is well-conditioned and can be solved by any standard matrix inverter. For ill-posed problem, the matrix becomes ill-conditioned and the proper solution can be found by a few specialized algorithms based on the Singular Value Decomposition (SVD) approach [21-25]. This method has been shown to suppress the amplification in measurement errors [13, 16, 17] in the input data, while both minimizing the variance in the predicted values and preventing output bias. This algorithm is applicable to complex, multiply-connected, two and three-dimensional configurations.

The main benefit of using the BEM together with the SVD algorithm is that it provides a very fast, robust, accurate, non-iterative, inverse boundary conditions determination methodology. The method is readily applicable on laptop personal computers.

AN EXAMPLE OF THE NUMERICAL FORMULATION

A brief analytical and numerical formulation using BEM will be demonstrated in the case of steady heat conduction, although the formulation is similar in the case of other field problems [18-20]. The heat conduction equation for the steady-state temperature distribution, $T(\mathbf{x})$, in a solid isotropic domain Ω bounded by the boundary Γ is given by

$$\nabla \bullet \left[k(T)\, \nabla T(\mathbf{x})\right] + L(\mathbf{x}) = 0 \qquad (1)$$

Here, $k(T)$ is the temperature-dependent coefficient of thermal conductivity, $\mathbf{x}$ is the position vector, and $L(\mathbf{x})$ is a function representing arbitrarily distributed heat sources (or sinks) per unit volume. This quasi-linear elliptic partial differential equation can be subject to the Dirichlet (temperature, T) boundary conditions on some parts of the boundary, the Neumann (heat flux, Q) boundary conditions on the other parts of the boundary, radiation heat flux conditions on yet another part of the boundary, and, when a boundary is exposed to a moving fluid, the Robin (convective heat transfer) boundary conditions on the remaining boundary, Γ_{conv},

$$-k\left.\frac{\partial T}{\partial n}\right|_{\Gamma_{conv}} = h_{conv}\left(\left.T\right|_{\Gamma_{conv}} - T_{amb}\right) \qquad (2)$$

Here, n is the direction of the outward normal to the boundary, h_{conv} is the local convective heat transfer coefficient, and T_{amb} is the ambient fluid temperature. Kirchhoff defined the non-dimensional temperature, $\Theta(\mathbf{x})$, as

$$\Theta(\mathbf{x}) = \int_{0}^{T} \frac{k(T)}{k_o} \frac{dT}{(T_{max} - T_{min})} \qquad (3)$$

where k_o = constant is the reference coefficient of thermal conductivity. The Equation (1) then becomes Poisson's equation for the non-dimensional temperature

$$\nabla^2\Theta(\mathbf{x}) + f(\mathbf{x}) = 0 \qquad (4)$$

Here, the non-dimensionalized distributed heat sources function is defined as

$$f(\mathbf{x}) = \frac{L(\mathbf{x})}{k_o} \frac{\ell^2}{(T_{max} - T_{min})} \qquad (5)$$

where ℓ is the characteristic length. The Neumann boundary conditions can be transformed in terms of Kirchhoff's non-dimensional flux, $\bar{q}$, as

$$\bar{q} = \frac{\partial \overline{\Theta}}{\partial n} \qquad (6)$$

In addition, if the domain, Ω, is heterogeneous, it may be subdivided into a number of subdomains each having a different coefficient of thermal conductivity. The solutions to Eq. (4) for each subdomain are then combined equating temperatures and heat fluxes on the interface boundaries [12].

The BEM is a non-iterative solution procedure which, when used for linear boundary condition problems, is significantly faster and more robust than the other numerical solution techniques. In addition, the non-iterative nature of the BEM eliminates stability, numerical dissipation and convergence problems, as well as removing any need for artificial dissipation. Analytical solutions to the partial differential equation, in the form of the Green's function, are part of the BEM solution. Therefore, high accuracy is expected because introducing the Green's functions does not introduce any error into the solution. This is valuable because iterative inverse problem solving procedures tend to amplify errors thus requiring complex regularization (smoothing) algorithms [11].

We will sketch the BEM in case of the Laplace equation. The BEM starts with Green's second identity which is equivalent to integrating the weighted residual statement by parts twice [19, 20]

$$\int_{\Omega}\left(\nabla^2 T u^* - T\nabla^2 u^*\right)d\Omega = \int_{\Gamma}\left(\frac{\partial T}{\partial n}u^* - T\frac{\partial u^*}{\partial n}\right)d\Gamma \qquad (7)$$

where the fundamental solution, u^*, is the solution to the adjoint of the governing partial differential equation which satisfies the homogeneous boundary conditions in an infinite domain [26]. After retaining the Cauchy principal value of the boundary integrals, and using the properties of the Dirac delta function, the following boundary integral equation is obtained [20]

$$c(x)T(x) + \int_{\Gamma} q^*(x,\xi)T(\xi)d\Gamma = \int_{\Gamma} u^*(x,\xi)q(\xi)d\Gamma \quad (8)$$

Since we are strictly solving a boundary condition problem, the unknown temperature T(**x**) is on the boundary Γ_{conv} which is a part of the overall boundary Γ. The boundary Γ can be discretized into N_{BE} isoparametric boundary elements connected at N_{BN} boundary nodes. In addition, N_{INT} internal measurement points could exist where temperature data is obtained. The T and q can vary between the neighboring end-nodes defining each boundary element, each boundary element is integrated numerically using a standard Gaussian quadrature integration formula. Boundary elements containing a singularity at one end-point can be integrated analytically resulting in a set of $N_{BN}+N_{INT}$ boundary integral equations, one for each boundary node plus one for every internal temperature measurement. The resulting discretized form of the BEM can be represented in matrix form as

$$[H]\{U\} = [G]\{Q\} \quad (9)$$

where **[H]** and **[G]** are the geometric coefficient matrices. For a well-posed boundary condition problem, every point on the boundary is given one Dirichlet, Neumann or Robin boundary condition and no internal temperature measurements. These boundary conditions are then multiplied by their respective coefficient matrix and collected on the right hand side to form a vector of known values, **{F}**. The left-hand side remains in the standard form **[A]{X}**. This well-posed system of linear algebraic equations can be solved for the vector of unknown values **{X}** on the boundary by any standard matrix solver such as Gaussian elimination or LU factorization. The entire procedure can similarly be formulated for Poisson equation and other field equations [12, 18-20].

If the boundary conditions (T, q, or h_{conv}) are unknown on parts of the boundary or if internal temperature measurements are included in the analysis, the problem becomes ill-posed. A solution may still be obtained by multiplying the known quantities in the vectors **{U}** and **{Q}** by their respective coefficient matrix columns and collecting them into the vector of knowns, **{F}**. The unknowns form a single vector, **{X}**, multiplied by a highly ill-conditioned coefficient matrix, **[A]**, which is, in general, not square. The truncated Singular Value Decomposition (SVD) method [21-25] has been often used to solve this ill-conditioned system of algebraic equations. In order to determine which singular values in **[A]** are to be truncated, we must choose a user-specified singularity threshold parameter, τ_{SVD}. Any singular value, whose ratio with the largest singular value is less than this singularity threshold, is zeroed out. Consequently, those algebraic terms that are dominated by noise and round-off error are eliminated from the matrix.

Tikhonov's regularization [8] is another type of single-parameter minimization where the solution vector **{X}** minimizes the weighted sum of the norm of the error vector plus a penalty term. Tikhonov's regularization is a generalization of least-squares truncation. Instead of simply eliminating terms associated with small singular values, they are weighted by a factor $(1 + \tau_{TIH} / \omega^2)$ where ω is any of the singular values of the matrix **[A]**. The Tikhonov's regularization parameter, τ_{TIH}, plays an important role. A low value drives the residual term **[A]{X}-{F}** smaller, approaching the least squares solution. Because of the destabilizing effect of the small singular values, the solution for an ill-conditioned matrix often oscillates erratically. Larger Tikhonov's regularization parameters act as a filter to gradually reduce the effect of the singular values because ω_j/ω_{max} are less than the regularization parameter, τ_{TIH}. Thus, the optimal choice of the regularization parameter provides a balance between the accuracy and the smoothness of the solution and it should be chosen very carefully [13].

We have performed detailed testing of both SVD and Tikhonov's regularization in a number of test cases involving heat conduction inverse boundary condition problems [12, 13]. Contrary to the widely accepted beliefs, we observed that Tikhonov's regularization produces smooth results but often generates unacceptable levels of global error [13].

EXAMPLES OF NUMERICAL RESULTS

We will first demonstrate the performance of our non-iterative BEM inverse code on a rectangular plate (Fig. 1) that was subject to homogeneous Dirichlet boundary conditions (T = 0 °C) on three boundaries and a Robin boundary condition (h_{conv} = 1.0 W/m^2 °C, T_{amb} = 1.0 °C) on the bottom boundary.

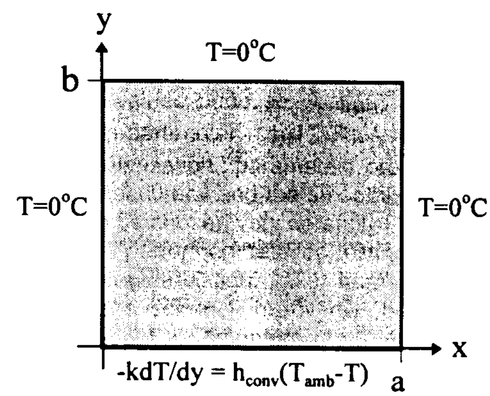

Fig. 1 Rectangular plate with three homogeneous Dirichlet and one Robin boundary conditions.

An analytical solution for this well-posed problem can be found using separation of variables. The inverse problem was formulated by specifying nothing on the bottom boundary while the remaining boundaries were over-specified with temperatures and heat fluxes taken from the analytical solution. Heat conduction coefficient was uniformly k = 1.0 W/m °C. The four boundaries of the rectangular plate were discretized with 10 equal-length isoparametric linear boundary elements per side.

Convective heat transfer coefficients are difficult to obtain experimentally, because they depend strongly on at least twelve variables or eight non-dimensional groups [27]. Typical semi-empirical expressions for prediction of heat convection coefficients represent curve fits through experimental data for very simple configurations covering only limited ranges of flow-field parameters.

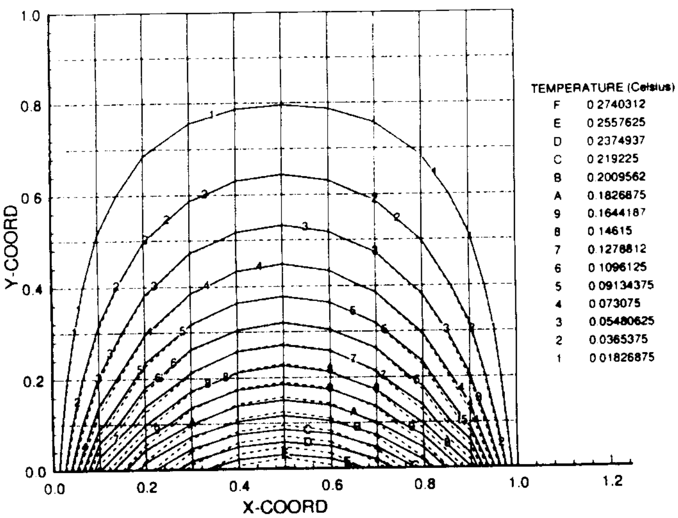

Fig. 2 Isotherms predicted within the rectangular plate by the analytical (solid lines), inverse BEM with top boundary over-specified (dashed lines), and the inverse BEM with top and side boundaries over-specified (dash-dot lines).

The most innovative aspect of this inverse BEM approach is that it does not require any information about the flow-field and that it is non-iterative. The equation for the heat flux from the Robin boundary condition was added directly into the linear BEM system. The unknown temperatures were factored together with the other nodal temperatures appearing on the left-hand side of the BEM matrix equation set. After the ill-conditioned coefficient matrix [A] has been inverted, the unknown boundary conditions of T and q were obtained from {X} = $[A]^{-1}$ {F}. Once these boundary conditions were known on the boundary Γ_{conv}, the convective heat transfer coefficients were determined from Eq. (2) since T_{amb} is considered as known.

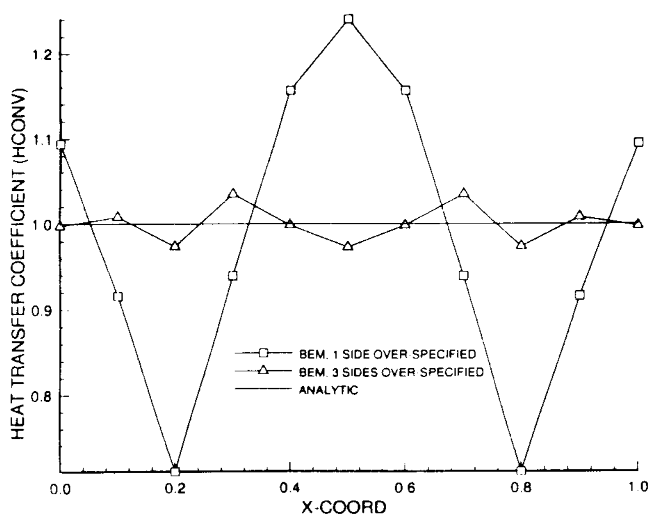

Fig. 3 Convective heat transfer coefficient numerically predicted by the inverse BEM on the square plate when the opposite boundary (squares) and three boundaries (triangles) were over-specified.

The computed temperature field (Fig. 2) and the computed convective heat transfer coefficients (Fig. 3) on the bottom boundary, which in this test case should be h_{conv} = 1.0 W/m^2 ^{o}C, indicate increase in accuracy with the increased amount of over-specified data and the decrease in distance between the over-specified and unspecified boundaries [13]. When repeated for a variety of practical Biot numbers (B_i = h_{conv} b / k), this method was found (Fig. 4) to be reliable and very fast allowing realistic values of h_{conv} to be predicted [16].

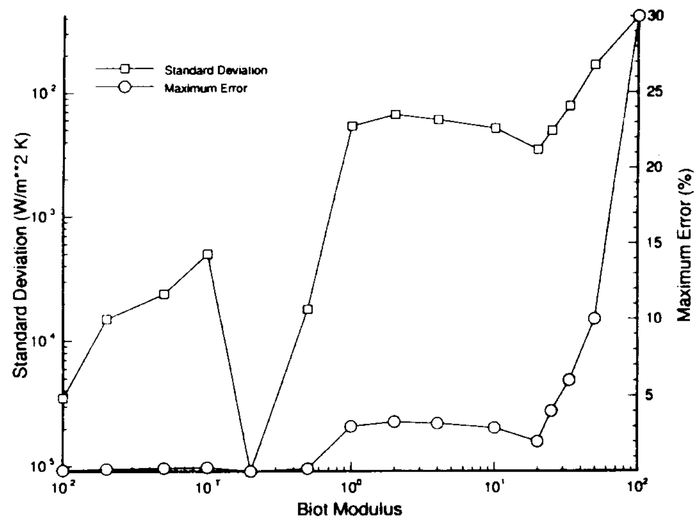

Fig. 4 Influence of Biot number on maximum error and standard deviation of the predicted values of h_{conv}.

Even more accurate results were obtained in the case when the bottom boundary was specified with variable (Fig. 5) heat convection coefficient $h_{conv} = 1.0 + \sin(2\pi x)$ thus confirming the applicability of this inverse BEM algorithm to prediction of variable h_{conv} values.

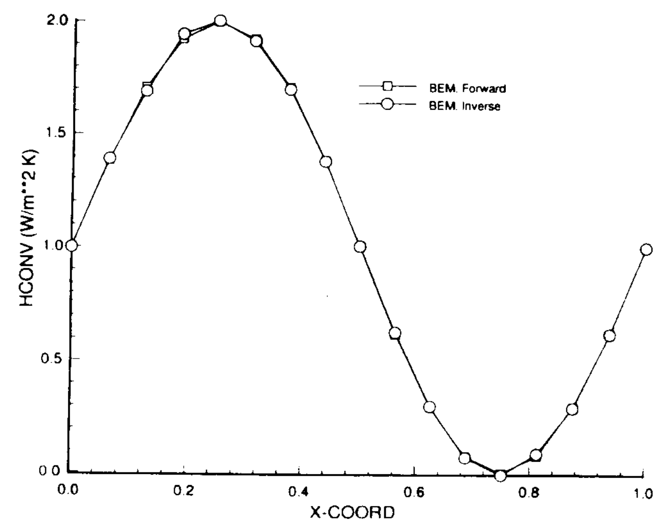

Fig. 5 Exact (squares) and inverse BEM predicted (circles) variation of h_{conv} on the bottom boundary.

A very high accuracy in predicting unknown boundary has been demonstrated in multiply-connected two-dimensional annular domains for heat conduction problems without and with arbitrary distributed heat source function [13] and in linear elastostatics [18]. The inverse BEM has also been demonstrated on three-dimensional objects like multiply-coated rocket engine nozzles [12, 14] and a three-dimensional multiple-material electronic chip assembly with a heat sink [15].

Since heat flux measurement probes are orders of magnitude more expensive than the temperature measurement probes, our inverse BEM algorithm was also demonstrated [13] for the case where only temperature measurements were provided on a part of the multiply-connected (annular) domain. The over-specified data consisted of a small number of interior temperature measurements. The predicted temperatures and heat fluxes using this approach were very accurate.

Recently, the inverse BEM approach has been extended to non-destructive determination of temperature-dependent heat conductivity coefficients [17]. The method is also non-iterative and can be used in practical problems where the objects are arbitrarily shaped and sized.

The inverse BEM formulation was also demonstrated to work in finding unknown fluid temperatures at the exit boundary of a thermoviscous flow-field [28].

An earlier version of the unsteady BEM in conjunction with an optimization algorithm was successfully used in predicting proper unsteady variation of boundary temperatures and heat fluxes that are required to maintain the desired cooling rates inside the multiply-connected domain with direct application to cryobiology and material processing [29, 30].

SENSITIVITY TO MEASUREMENT ERRORS

The major concern of engineers dealing with inverse problems is the sensitivity and accuracy of their algorithms as a result of errors committed in measuring the boundary conditions.

In our test cases, this was numerically simulated by adding a random error based on the Gaussian probability density distribution to the temperature measurements. A random number $0 < R < 1$ was generated using a standard utility subroutine. The desired variance σ^2 was specified and error was added to the analytical temperature data points T according to

$$T_{perturb} = T \pm \sqrt{-2\sigma^2 \ln R} \qquad (10)$$

where addition and subtraction of the random error had a 50-50 chance of been chosen. This simple test

It can be seen (Fig. 6) that the average error in the predicted h_{conv} is of the approximately same magnitude as the average level of the errors introduced in the over-specified boundary temperatures. Most of the iterative inverse boundary condition determination algorithms cause significantly larger errors in the predicted values than the errors introduced in the specified boundary conditions. This means that our non-iterative inverse BEM algorithm does not have a need for the sophisticated regularization algorithms [8-11].

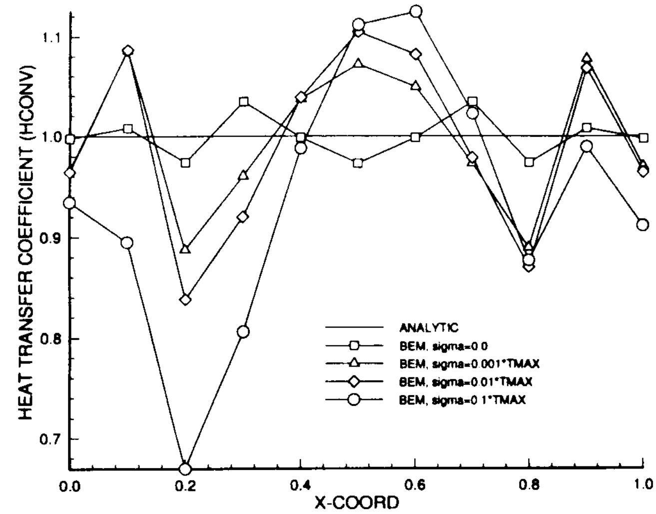

Fig. 6. **Sensitivity of the predicted convective heat transfer coefficient distributions for different standard deviations of the over-specified boundary temperatures.**

CONCLUSIONS

Using a simple example of boundary value problems governed by the Laplace equation, we have demonstrated how a simple modification to any existing non-iterative BEM analysis algorithm can transform it into an inverse non-iterative code for prediction of unknown distributions of steady boundary conditions. This method is applicable to arbitrarily shaped two and three-dimensional solids where at least part of a boundary can be over-specified with both the field variable and its normal derivative. The method is extremely fast and robust since it requires inversion of a single fully populated matrix. This method is considerably less sensitive to the errors introduced in the boundary measurements of temperature than are the general iterative inverse methods.

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