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INVERSE DETERMINATION OF SPATIALLY VARYING DIFFUSION COEFFICIENT IN TWO-DIMENSIONAL OBJECTS

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Abstract

Coefficients of thermal conductivity, magnetic permeability or electric permittivity can vary spatially throughout a given solid object. Finding this spatial variation of such a diffusion coefficient is an inverse problem that requires measurements of boundary values of the diffused field quantity such as temperature, magnetic field potential or electric field potential and its derivatives normal to the boundaries. The method for determining the unknown spatial distribution of diffusion coefficient presented here is based on numerically predicting the spatial distribution of the field variable based on its measured boundary values and on the assumed spatial distribution of the diffusion coefficient. The direct problem was solved using radial basis functions formulation whose accuracy was verified against analytical solutions. The minimization of the normalized least squares difference between the calculated and measured values of the diffused field quantity at the boundaries then leads to the correct spatial distribution of the coefficient of diffusion. Minimization was performed using our hybrid single objective optimization algorithm. Results of this approach to inverse determination of spatially varying diffusivity coefficient were verified against an analytical solution.

INTRODUCTION

This paper deals with determination of spatially varying diffusive properties of media using steady boundary measurements of field quantities [1]. Examples of such problems are determination of spatially varying thermal conductivity, electric permittivity, magnetic permeability, *etc.* This can be used in cases when trying to detect subdomains inside a given object that might be made of different materials. On the other hand, this method can be used in the design of functionally graded materials achievable using additive manufacturing for objects with fixed geometry and desired boundary values of the field quantity. Such problems are mathematically modeled by an elliptic partial differential equation governing the steady diffusion of a solenoidal field quantity ϕ in a solid.

$$\nabla \bullet (\lambda \nabla \phi) = 0 \tag{1}$$

Here, $\phi = \phi(x, y)$ is a passive scalar that can be the absolute temperature, the electric field potential, the magnetic field potential, the concentration of certain dopants or impurities diffused in a solid, *etc.* Correspondingly, the diffusivity coefficient, λ, can be thermal conductivity, electric permittivity, magnetic permeability, dopant diffusion coefficient, *etc.* Since $\lambda = \lambda(x, y)$ is a scalar quantity, equation (1) can be expressed, in the case of a two-dimensional solid, as

$$\frac{\partial}{\partial x}(\lambda \frac{\partial \phi}{\partial x}) + \frac{\partial}{\partial y}(\lambda \frac{\partial \phi}{\partial y}) = 0 \tag{2}$$

The question is: If values of ϕ or its normal derivative are given on the boundaries of the solid object, how can the spatial distributions of the diffusion coefficient, λ, be determined in order to satisfy equation (1) subjected to these boundary conditions?

In the case of an analysis problem, the spatial distribution of ϕ is uniquely determined by numerically integrating Eq. 1 subject to given size and shape of the domain, spatial distribution of λ, and either Dirichlet or Neumann boundary condition at every point of the boundary.

In the case of an inverse problem of determining unknown spatial distribution of λ, there is a need for additional information compensating for the lack of knowledge of λ. This additional information is given in the form of over-specified boundary conditions. Specifically, both Dirichlet and Neumann boundary conditions should be given at as many as possible boundary points. That is, over-specified data is required, such as the values of both ϕ and $\partial\phi/\partial n$ on the boundaries are given, or internal measurements of ϕ are given, or a combination of boundary and internal data are given. For practical reasons, measurements of ϕ at internal points are not commonly used.

The inverse problem of determining spatially-dependent material properties of the material will be solved using a two-stage approach. First, this is a very difficult problem if this spatial dependence is random, that is, if it does not have a simple continuous functional description. If this is the case, then a large amount of internal measurements of ϕ will be required. The problem is more tractable if some *a priori* information about the material property spatial variations is known (that is, the material property is known to vary as a function of *x,y* such that the variation belongs to a family of basis functions).

If some functional description for variation of ϕ is available, then the easiest way to solve the problem is to use an optimization, root finding or least squares algorithm to minimize the difference between the computed ϕ or $\partial\phi/\partial n$ on the boundaries (or computed values of ϕ inside the domain at the internal measurement locations) and specified data (measured $\partial\phi/\partial n$ on the boundary or ϕ at internal measurement points). This iterative algorithm would attempt to find the coefficients of the basis functions of $\lambda(x,y)$. Here, the coefficients of the basis functions (Chebyshev polynomials, beta-splines, Fourier series, etc.) are the design variables of the least squares minimization algorithm.

If only values of ϕ and $\partial\phi/\partial n$ on the boundaries are available, then the inverse method will only be able to predict linear variations of λ with respect to *x,y,z*. In other words, the inverse method will only be able to identify up to 3 basis function coefficients (linear, $A + x$, $B + y$, $C + z$).

AN ANALYTICAL SOLUTION FOR SPATIALY VARYING THERMAL CONDUCTIVITY

Thermal conductivity coefficient, k, is one of the most commonly studied and utilized diffusion coefficients. It is most often treated as a constant or a temperature-dependent quantity $k = k(T)$ in which case it can be accurately determined using Kirchoff's transformation [2].

In a growing field of design of functionally graded materials, it is an imperative to create spatially varying thermo-physical properties that will assure desired non-isotropy, thus functionality, of such materials and objects made using additive manufacturing processes. In this paper, we will focus on using only steady-state temperature fields and steady-state thermal boundary conditions.

So, the question is: for a pre-specified steady temperature field distribution in a solid object, what should be the spatial variation of thermal conductivity in this object that will create such a desired temperature field?

Initially, computer code verification is needed, in order to check the capability of the method to solve a problem accurately for spatially varying diffusion coefficient. The verification was made against an analytical solution.

For example, if thermal conductivity distribution in a two-dimensional rectangular domain is given as

$$k(x,y) = (A + x)(B + y) \tag{3}$$

where A and B are arbitrary constants, then the governing analytical solution for temperature field should have the general form

$$T(x,y) = (A + x)^2 - (B + y)^2 \tag{4}$$

which satisfies the governing steady heat flux balance equation

$$0 = \frac{\partial}{\partial x}(k\frac{\partial T}{\partial x}) + \frac{\partial}{\partial y}(k\frac{\partial T}{\partial y}) = \frac{\partial k}{\partial x}\frac{\partial T}{\partial x} + \frac{\partial k}{\partial y}\frac{\partial T}{\partial y} + k\left(\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2}\right) \quad (5)$$

For this general analytical solution for temperature field, values of the corresponding temperatures and temperature derivatives on the boundaries of a domain must be given.

Spatially varying thermal conductivity, k, can then be determined from the over-specified thermal boundary conditions using Bayesian statistics employing Kalman filters or non-linear filters [3,4].

However, an entirely different approach to inverse determination of spatially varying physical properties of media is based on a combination of a field analysis algorithm (which can be based on finite differencing, finite volumes, finite elements, boundary elements, etc.) or experimental data and a minimization algorithm that is either gradient based or non-gradient based or a hybrid of the two [5].

Radial Basis Functions (RBFs) are essential ingredients of the techniques generally known as "meshless methods". In one way or another, all meshless techniques require some sort of distance measure to evaluate the influence of a given location on another part of the domain.

The use of RBFs followed by collocation, a technique first proposed by Kansa [8], after the work of Hardy [6] on multivariate approximation, is now becoming an established approach and various applications to problems of structures and fluids have been made in recent years [7].

RBF method (or asymmetric collocation) starts by building an approximation to the field of interest (normally displacement components) from the superposition of RBFs (globally or compactly supported) conveniently placed at points in the domain and, or, at the boundary.

The unknowns, which are the coefficients of each RBF, are obtained from the (approximate) enforcement of the boundary conditions as well as the governing equations by means of collocation. Usually, this approximation only considers regular radial basis functions, such as the globally supported multiquadrics or the compactly supported Wendland functions.

In this paper, the temperature is represented using RBFs as

$$T(x,y) = \sum_{i=1}^{N} \psi_i \phi(\mathbf{r}_i) \quad (6)$$

where

$$\phi(x,y) = \left[(x - x_i)^2 + (y - y_i)^2 + c^2\right]^{\omega} \quad (7)$$

Thus, equation (5) becomes a linear system for the unknown coefficients ψ, if the conduction coefficient, k, and the boundary conditions are known. In the case of an inverse problem, since the values of A and B in equation (3) are not known, such system has to be solved by a minimization technique.

We first tested the accuracy of the numerical integration algorithms for the case where constants A and B were both equal to 1.0. For this test case, figures 1-4 depict 176 symmetrically clustered collocation points used for a RBF expansion of the temperature appearing in governing equation (5), analytical distribution of the coefficient of thermal conductivity according to equation (6), the analytical temperature field given by equation (4), and RBF numerical solution for the temperature field, respectively.

It is worthwhile to notice (Figure 5) that relative numerical error in this test case is below one percent in the entire domain. Consequently, the RBF code used to numerically obtain the temperature field (equation 6) for a given distribution of k(x,y) (equation 3 with A = B = 1.0) was deemed sufficiently accurate for the purpose of performing inverse determination of the unknown distributions of k(x,y).

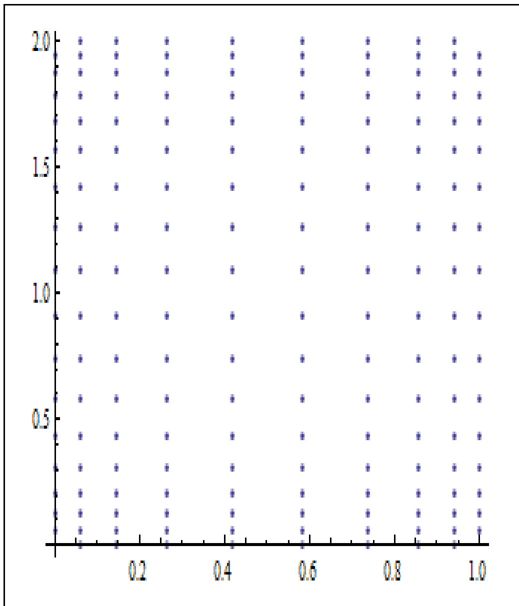

Figure 1. RBF collocation points used.

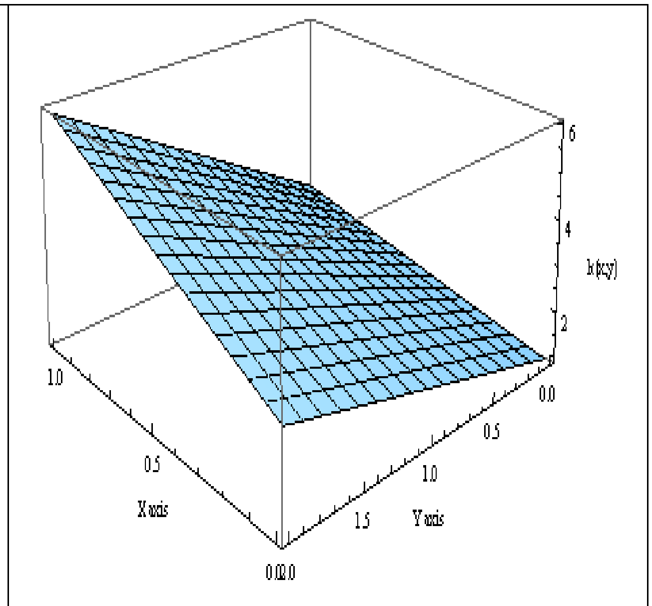

Figure 2. Analytical distribution of thermal conductivity.

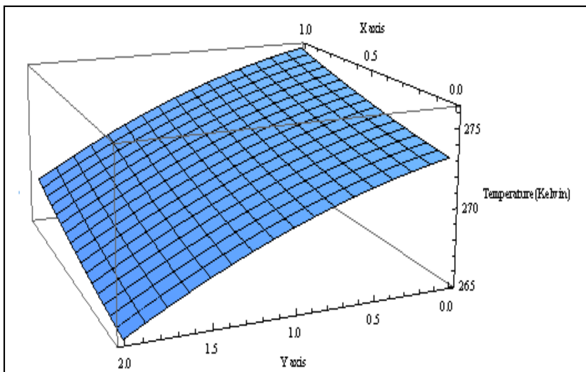

Figure 3. Analytical solution for T(x,y).

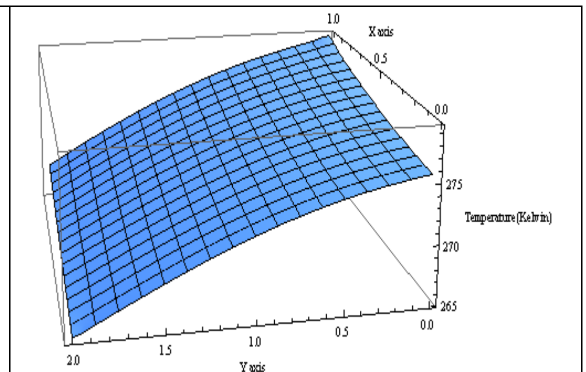

Figure 4. RBF numerical solution for T(x,y).

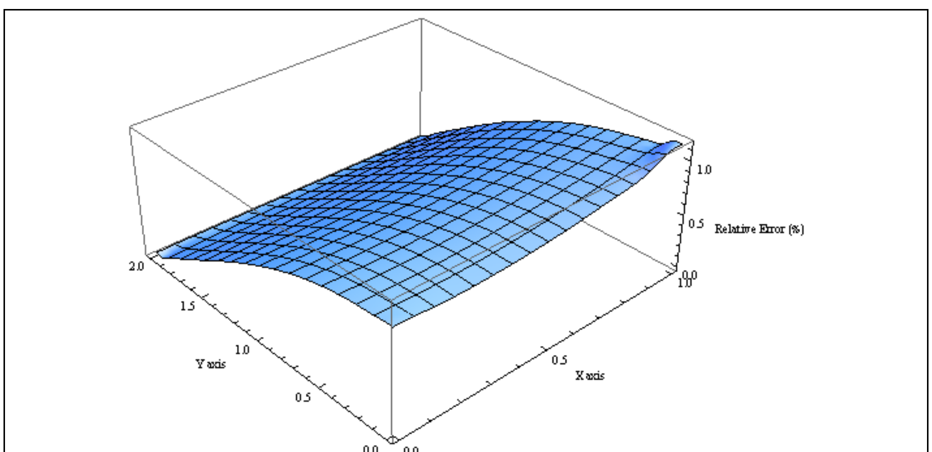

Figure 5. Relative error (in percents) distribution created by the RBF solution.

INVERSE DETERMINATION OF k(x,y) FROM THERMAL BOUNDARY CONDITIONS

The method used in this work to determine unknown spatial distribution of thermal conductivity k(x,y) is based on utilizing steady state values of temperatures and/or normal temperature derivatives (Dirichlet or Neumann boundary conditions) on boundaries of the domain. One can also use measurements of temperature inside the domain, but this approach is deemed to be too cumbersome, expensive and even impossible in many practical applications because it is not non-destructive.

Thus, for each choice of coefficients A and B subject to primary boundary conditions given in Table 1 and Table 2, RBF calculated the corresponding temperature field by solving the linear system resulting from the use of equation (6) into equation (5). The test example object was a rectangular domain $x\in[0,1]$ and $y\in[0,2]$ with analytical boundary conditions resulting from equation 4 given in Table 1 and Table 2.

Table 1. Analytical boundary conditions for test case no. 1 on bottom and top surfaces

	Bottom surface (y = 0.0 m)	Top surface (y = 2.0 m)
Primary boundary condition	$\frac{dT}{dy}=-2B$	$T(x,2)=(A+x)^2-(B+2)^2$
Secondary boundary condition	$T(x,0)=(A+x)^2-B^2$	$\frac{dT}{dy}=-2(B+2)$

Table 2. Analytical boundary conditions for test case no. 1 on left and right boundaries

	Left surface (x = 0.0 m)	Right surface (x = 1.0 m)
Primary boundary condition	$\frac{dT}{dx}=2A$	$\frac{dT}{dx}=2(A+1)$
Secondary boundary condition	$T(0,y)=A^2-(B+y)^2$	$T(1,y)=(A+1)^2-(B+y)^2$

As a byproduct of this numerical analysis, secondary boundary conditions were also calculated.

For the purpose of the demonstration of the entire process, let us treat the analytical values of the secondary boundary conditions (Tables 1 and 2) as “measured” boundary values. They correspond to one particular distribution of thermal conductivity given by equation (3).

Now, let us pretend that we do not know that A = B = 1.0 values in the model for spatial distribution of k(x,y) given by equation (3) are the correct values that have generated this analytical solution for temperature field and its secondary boundary conditions (“measured” boundary values).

So, if we guess certain values for coefficients A and B and use them in primary boundary conditions to solve equation (5) using RBF, we will get some “calculated” temperature field and some “calculated” secondary boundary conditions which will be different than the “measured” values of the secondary boundary conditions [8].

The sum of least squares of all differences between calculated and “measured” (in our example case this means analytical) values of boundary temperatures (normalized with the total number of boundary points involved, N_{tot}) is the functional J that needs to be minimized in order to determine the values of A and B that satisfy the governing equation (5) and the “measured” boundary conditions. This functional J is given as

$$J = \begin{bmatrix} \sum_{j=1}^{j\max} \left[\left(T_j^{calc} - T_j^{meas} \right) / \left(T_j^{meas} + \varepsilon \right) \right]_{x=x_{\min}}^2 \\ + \sum_{j=1}^{j\max} \left[\left(T_j^{calc} - T_j^{meas} \right) / \left(T_j^{meas} + \varepsilon \right) \right]_{x=x_{\max}}^2 \\ + \sum_{i=1}^{i\max} \left[\left(T_i^{calc} - T_i^{meas} \right) / \left(T_i^{meas} + \varepsilon \right) \right]_{y=y_{\min}}^2 \end{bmatrix} \tag{8}$$

where ε is a small parameter of the order 0.00001

In this simple example case given by equations 5 and 6, this task will thus be a single-objective optimization with two design variables (A and B).

Minimization of the functional *J* can be performed with any single-objective robust minimization algorithm [9], while bounding the search range for each design variable as -100.00 < A < 100.00 and -100.00 < B < 100.00. The minimization algorithm converged to values A = 0.99207 and B = 0.998314, while relative errors in the corresponding temperatures were below one percent.

INVERSE DETERMINATION OF HIGH GRADIENT THERMAL CONDUCTIVITY

In the second test case, we did not use an analytical solution in lieu of "measured" temperature field and the corresponding "measured" boundary conditions. Instead, for demonstration purposes only, we specified the following high gradient variation of thermal conductivity

$$k(x,y) = k_{\min} + \left(k_{\max} - k_{\min} \right) \left[x - \frac{A}{2\pi} \sin(2\pi x) \right] \left[y - \frac{B}{2\pi} \sin(\pi y) \right] \tag{9}$$

where 0.00 < A < 0.99 and 0.00 < B < 0.99.

A "measured" solution was created by integrating equation 5 with this distribution of thermal conductivity (equation 9 with $k_{\min} = 200.00 \text{ W K}^{-1}\text{m}^{-1}$ and $k_{\max} = 5000.00 \text{ W K}^{-1}\text{m}^{-1}$) using RBF. Table 3 shows the boundary conditions used in this integration.

Table 3. Analytical primary boundary conditions for test case no. 2

Bottom surface (y = 0.0 m)	Top surface (y = 2.0 m)	Left surface (x = 0.0 m)	Right surface (x = 1.0 m)
$T = 85.00 \text{ K}$	$\frac{dT}{dy} = 600 \text{ K m}^{-1}$	$\frac{dT}{dx} = 10.00 \text{ K m}^{-1}$	$\frac{dT}{dx} = 10.00 \text{ K m}^{-1}$

Figures 6 and 7 show spatial variation of thermal conductivity according to equation (9) and temperature field calculated using RBF and boundary conditions given in Table 3 with the indicated values for minimum and maximum thermal conductivities. Coefficients in equation (9) were given as A = B = 0.85.

The secondary thermal boundary conditions (temperature distributions on left, top, and right walls) were then calculated as a byproduct of the RBF integration of equation (5). These calculated secondary boundary conditions (wall temperature distributions) were then treated as "measured" values of the boundary temperatures.

We fully understand that this process (using the same code to calculate the "measured" boundary conditions and to calculate "calculated" boundary conditions when guessing the spatial distribution of thermal conductivity, constitutes a cardinal "inverse crime". However, for the purpose of demonstrating the basic concept and its robustness and versatility, we have decided to use the calculated secondary boundary conditions as the "measured" boundary conditions.

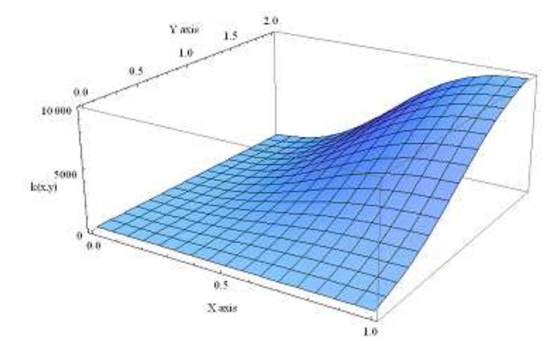

Figure 6. Actual distribution of thermal conductivity for case 2 (equation 13).

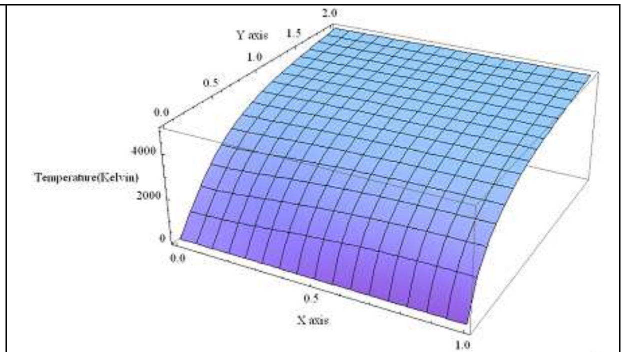

Figure 7. RBF numerical solution for T(x,y) subject to equation (13) and Table 3.

Minimization of the functional J (equation 8) for test case 2 was then performed by using particle swarm minimization [9] with response surface [10] to find the proper values of the four variables in these ranges:

$100.00 < k_{min} < 300.00$ $\qquad$ $0.00 < A < 0.95$

$1000.00 < k_{max} < 6000.00$ $\qquad$ $0.00 < B < 0.95$

The particle swarm optimizer converged to the following values of these four variables after 20 generations using RBF integrations of equation (6) and using a population of 50 particles.

Table 4. Convergence history of the optimization process for test case 2

Generation	k_{min}	k_{max}	A	B
1	184.015	4576.262	0.793	0.850
5	185.893	4623.601	0.882	0.857
10	185.475	4622.858	0.866	0.852
15	185.307	4624.883	0.853	0.853
20	185.307	4624.883	0.853	0.853

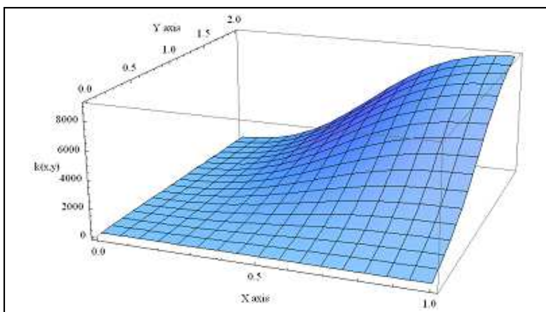

Figure 8. Thermal conductivity distribution using optimized four coefficients.

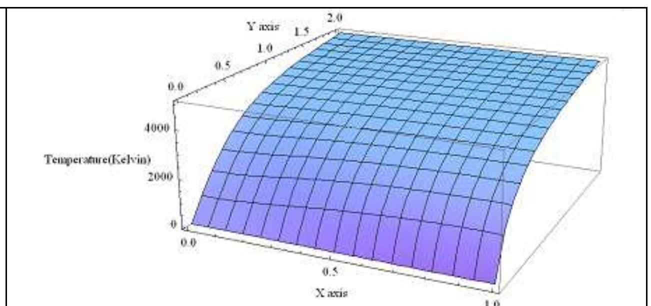

Figure 9. Temperature field calculated using the optimized four coefficients.

The coefficients k_{min} and k_{max} are not fully converged indicating a possibility that the basic particle swarm algorithm converged to a local minimum. This can be remedied by using a robust hybrid optimization algorithm [5,9] and more accurate response surface algorithm [10].

Spatial distribution of inversely obtained thermal conductivity (Figure 8) and its corresponding temperature field (Figure 9) closely resemble the exact distributions given in Figures 6 and 7, respectively.

CONCLUSIONS

Inverse determination of continuously varying thermal conductivity in arbitrary two-dimensional domains can be accurately determined using minimization of the least squares norm between calculated thermal boundary conditions (with guessed detailed spatial distributions of thermal conductivity) and measured thermal boundary conditions. A Radial Basis Function algorithm was used for numerical integration of the quasi-linear elliptic partial differential equation governing steady temperature distribution. Particle swarm optimization algorithm with a response surface was used for minimization of the normalized sum of least squares differences between calculated and measured thermal boundary conditions. Future efforts in identification of spatially distributed physical properties will focus on three-dimensional applications and on basis functions involving Fourier series that are capable of accurately modeling extreme gradients in the spatial variations of such coefficients. Optimization will be performed with hybrid optimization algorithms involving automatic switching among constituent modules.

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