4th *Inverse Problems, Design and Optimization Symposium* (IPDO-2013)
Albi, France, June 26-28, 2013

INVERSE DETERMINATION OF SPATIALLY VARYING THERMAL CONDUCTIVITY IN TWO-DIMENSIONAL OBJECTS

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Abstract
A general formulation for inverse determination of an arbitrarily spatially distributed diffusion coefficient, such as thermal conductivity, in a solid object has been developed and demonstrated in the case of a two-dimensional object. This is an inverse problem that requires some extra information, such as measurements of boundary values of the diffused field quantity such as temperature and its derivatives normal to the boundaries. The direct problem was formulated using radial basis functions formulation whose accuracy was verified against analytical solutions. The minimization of the difference between the calculated and measured values of the diffused field quantity at the boundaries was performed using a heuristic, single objective optimization algorithm, based on the particle swarm optimization method. Results of the inverse determination of spatially varying thermal conductivity were verified against an analytical solution.

Nomenclature

A,B	constants in the spatial distribution of thermal conductivity
β	a constant
δ	diffusion limit
λ	spatially distributed diffusion coefficient
d	spatial dimensionality of the problem
h	spatially varying coefficient
k	thermal conductivity coefficient, W m^{-1} K^{-1}
n	normal direction to the boundary
S	a spatially distributed source
t	time, s
T	absolute temperature, K
U	a diffused field variable
x,y,z	Cartesian coordinates, m

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. In a general case, let us consider a parabolic partial differential equation modeling the unsteady diffusion of a quantity *U*.

$$\beta \frac{\partial U}{\partial t} = \nabla \bullet (\lambda \nabla U) - hU + S \quad (1)$$

Here, *U* is a passive scalar that can be the absolute temperature, the concentration of certain dopants or impurities diffused in a solid, etc. Assuming that diffusivity coefficient, λ, is a scalar quantity, equation (1) can be expressed, in the case of a three-dimensional solid, as

$$\beta\frac{\partial U}{\partial t}=\frac{\partial}{\partial x}(\lambda\frac{\partial U}{\partial x})+\frac{\partial}{\partial y}(\lambda\frac{\partial U}{\partial y})+\frac{\partial}{\partial z}(\lambda\frac{\partial U}{\partial z})-hU+S \tag{2}$$

where

$$U=U(x,y,z;t) \tag{3}$$

$$\lambda=\lambda(x,y,z) \tag{4}$$

$$h=h(x,y,z) \tag{5}$$

$$S=S(x,y,z) \tag{6}$$

If values of U are given on the boundaries and the source S is known everywhere, how can spatial distributions of λ be determined in order to satisfy equation (1) subjected to the given boundary conditions?

First, over-specified data is required, such as the values of both U and $\partial U/\partial n$ on the boundaries, internal measurements of U, or a combination of boundary and internal data. Since the inverse problem has spatially-dependent material properties, 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 U 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,z such that the variation belongs to a family of basis functions).

If only values of U and $\partial U/\partial n$ 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, $A + x$, $B + y$, $C + z$).

If some functional description for variation of U 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 U or $\partial U/\partial n$ on the boundaries (or computed values of U inside the domain at the internal measurement locations) and specified data (measured $\partial U/\partial n$ on the boundary or U at internal measurement points). This iterative algorithm would attempt to find the coefficients of the basis functions of $\lambda(x,y,z)$. Here, the coefficients of the basis functions (Chebyshev polynomials, beta-splines, Fourier series, etc.) are the design variables of the least squares minimization algorithm.

There is another, more complex, way to solve this problem. The governing equation (1) could be expanded to the following form:

$$\beta\frac{\partial U}{\partial t}=\frac{\partial\lambda}{\partial x}\frac{\partial U}{\partial x}+\frac{\partial\lambda}{\partial y}\frac{\partial U}{\partial y}+\frac{\partial\lambda}{\partial z}\frac{\partial U}{\partial z}+\lambda\frac{\partial^2 U}{\partial x^2}+\lambda\frac{\partial^2 U}{\partial y^2}+\lambda\frac{\partial^2 U}{\partial z^2}-hU+S \tag{7}$$

Here, the first three terms on the right-hand-side are treated as unknown source terms. The derivatives $\partial U/\partial x$, $\partial U/\partial y$, $\partial U/\partial z$ are unknowns in the system matrix (they can be solved for), and $\partial\lambda/\partial x$, $\partial\lambda/\partial y$, $\partial\lambda/\partial z$ are unknowns in the inverse problem. This then becomes a source identification inverse problem, but now, the unknown coefficients of $\partial\lambda/\partial x$, $\partial\lambda/\partial y$, $\partial\lambda/\partial z$ are placed in the system matrix and solved for non-iteratively. Singular Value Decomposition matrix solver must be used, with the singular values either truncated or weighted by Tikhonov's regularization parameter.

It should be pointed out that difficulties might arise when the following parameter becomes too large

$$\frac{r^2}{2^d \frac{\lambda}{h} \Delta t} > \delta \tag{8}$$

where Δt is the integration time step and r is the distance from the over-specified data. The condition number of the matrix gets too large whenever the diffusion limit of $\delta = 20$ is exceeded.

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. In this paper, we will focus on using only steady-state temperature fields and steady-state 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, a 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 domain is given as

$$k(x,y) = (A+x)(B+y) \tag{9}$$

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

$$T(x,y) = (A+x)^2 - (B+y)^2 \tag{10}$$

which satisfies the governing steady heat flux balance equation

$$0 = \frac{\partial}{\partial x}(k\frac{\partial T}{\partial x}) + \frac{\partial}{\partial y}(k\frac{\partial T}{\partial y}) = \frac{\partial k}{\partial x}\frac{\partial T}{\partial x} + \frac{\partial k}{\partial y}\frac{\partial T}{\partial y} + k\left(\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2}\right) \tag{11}$$

For this general analytical solution for temperature field, values of the corresponding temperatures and temperature derivatives on the boundaries of a rectangular domain $x \in [0,1]$ and $y \in [0,2]$ are 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	$T(0,y) = A^2 - (B+y)^2$	$T(1,y) = (A+1)^2 - (B+y)^2$

Spatially varying thermal conductivity can be determined from the over-specified thermal boundary conditions using Bayesian statistics employing Kalman filters or non-linear filters [3-5].

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.

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 measure 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 [6], after the work of Hardy [7] on multivariate approximation, is now becoming an established approach and various applications to problems of structures and fluids have been made in recent years [8, 9].

Kansa's 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

$$T(x,y) = \sum_{i=1}^{N} \psi_i \phi(\mathbf{r}_i) \tag{12}$$

where

$$\phi(x,y) = \left[(x-x_i)^2 + (y-y_i)^2 + c^2\right]^{\omega} \tag{13}$$

Thus, equation (11) becomes a linear system for the unknown coefficients ψ, if the diffusion coefficient and the boundary conditions are known. In the case of an inverse problem, since the values of A and B in equation (9) 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 (11), analytical distribution of the coefficient of thermal conductivity according to equation (9), the analytical temperature field given by equation (10), 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 11) for a given distribution of k(x,y) (equation 9 with A = B = 1.0) was deemed sufficiently accurate for the purpose of performing inverse determination of the unknown distributions of k(x,y).

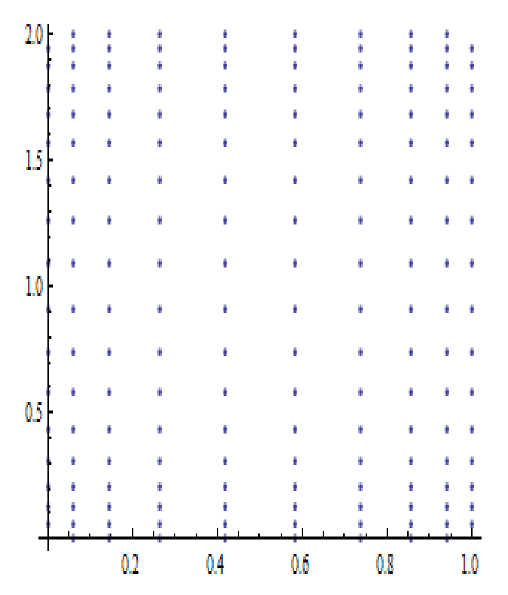

Figure 1. RBF collocation points used.

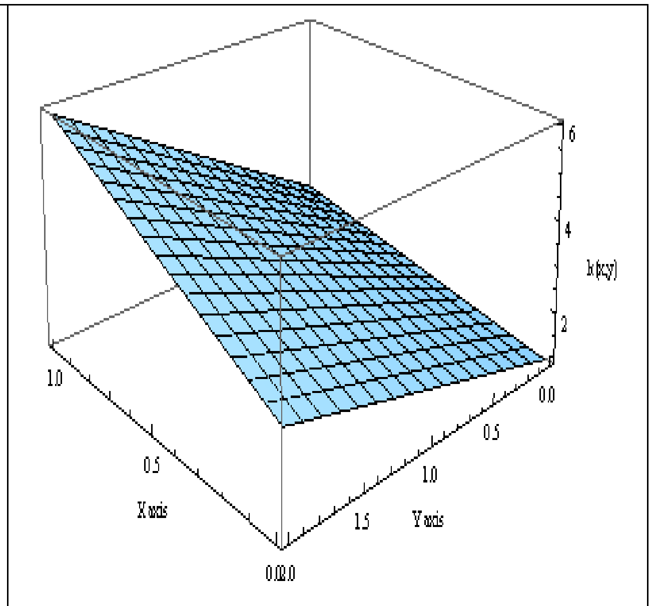

Figure 2. Analytical distribution of thermal conductivity.

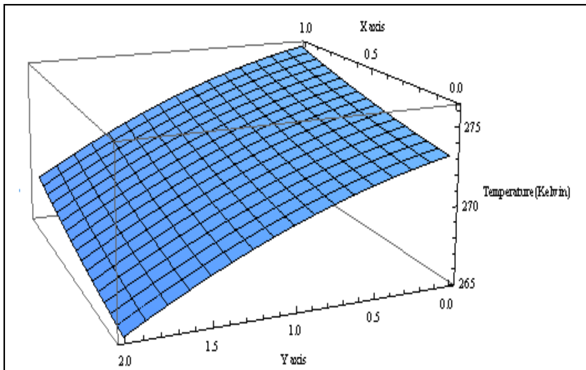

Figure 3. Analytical solution for T(x,y).

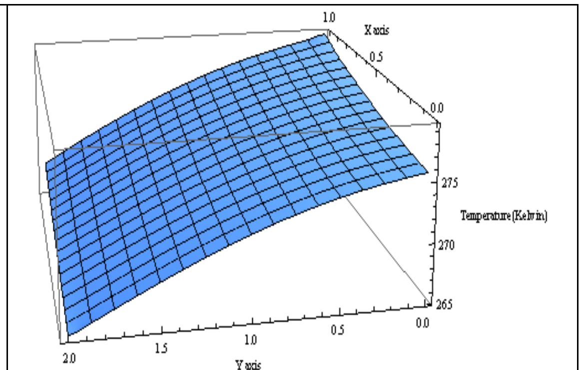

Figure 4. RBF numerical solution for T(x,y).

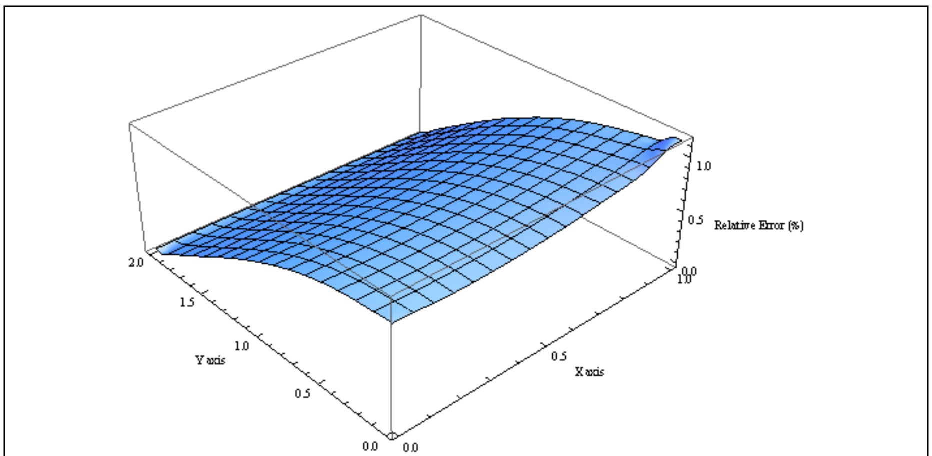

Figure 5. Relative error (in percents) distribution created by the RBF solution.

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 (12) into equation (11). 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 (see Tables 1 and 2) as “measured” values. They correspond to one particular distribution of thermal conductivity given by equation (9).

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 (9) 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 (11) 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.

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 (11) and the “measured” boundary conditions. This functional J is given as

$$J = \frac{1}{\mathrm{N_{tot}}}\left[\sum_{j=1}^{j\max}\left(T_j^{calc} - T_j^{meas}\right)^2_{x=x_{\min}} + \sum_{j=1}^{j\max}\left(T_j^{calc} - T_j^{meas}\right)^2_{x=x_{\max}} + \sum_{i=1}^{i\max}\left(T_i^{calc} - T_i^{meas}\right)^2_{y=y_{\min}}\right] \quad (14)$$

In this simple example case given by equations 9 and 10, 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 [10-12]. We utilized a standard version of particle swarm algorithm 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.

INVERSE DETERMINATION OF HIGH GRADIENT THERMAL CONDUCTIVITY

In this 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

$$k(x,y) = k_{\min} + \left(k_{\max} - k_{\min}\right)\left[x - \frac{A}{2\pi}\sin(2\pi x)\right]\left[y - \frac{B}{2\pi}\sin(\pi y)\right] \quad (15)$$

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

A “measured” solution was created by integrating equation 11 with this distribution of thermal conductivity (equation 15 with $k_{\min} = 200.00\ \mathrm{W\,K^{-1}m^{-1}}$ and $k_{\max} = 5000.00\ \mathrm{W\,K^{-1}m^{-1}}$) 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)
$T = 85.00$ K	$\frac{dT}{dy} = 600$ K m^{-1}	$\frac{dT}{dx} = 10.00$ K m^{-1}	$\frac{dT}{dx} = 10.00$ K m^{-1}

Figures 6 and 7 show spatial variation of thermal conductivity according to equation (15) and temperature field calculated using RBF and boundary conditions given in Table 3 with the indicated values for minimum and maximum thermal conductivities. Coefficients A and B in equation (15) were given as 0.85.

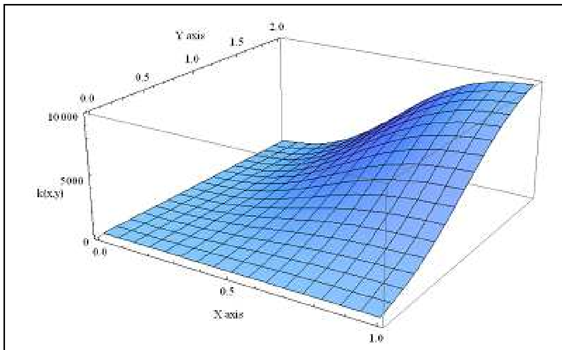

Figure 6. Actual distribution of thermal conductivity for case 2 (equation 13).

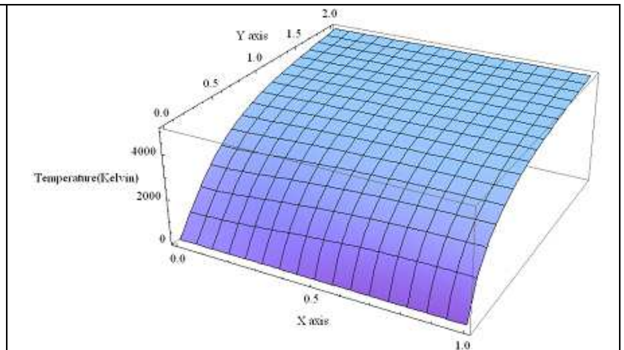

Figure 7. RBF numerical solution for T(x,y) subject to equation (13) and Table 3.

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 (11). 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.

Minimization of the functional J (equation 14) was then performed by using particle swarm minimization algorithm 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 (11) and using a population of 50 particles.

Table 4. Converge history of the particle swarm optimization process

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

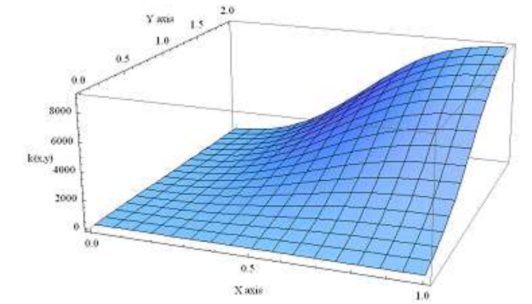

Figure 8. Thermal conductivity distribution using optimized four coefficients.

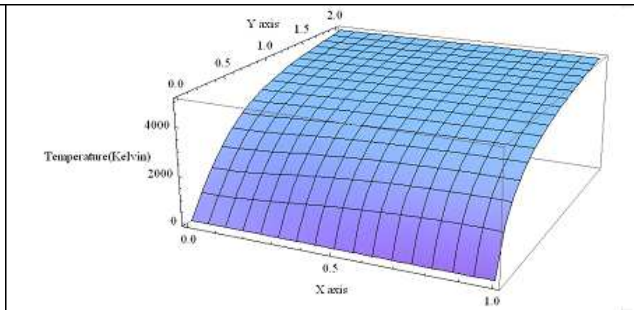

Figure 9. Temperature field using the optimized four coefficients.

The coefficients k_{min} and k_{max} are not fully converged indicating a possibility that the basis particle swarm algorithm converged to a local minimum. This can be remedied by using a robust hybrid optimization algorithm [10-12].

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 because it can easily and accurately predict temperature fields on arbitrary two-dimensional domains. Particle swarm optimization algorithm was used for minimization of the least squares norm because it is a robust evolutionary type algorithm that does not need gradients of the objective function and converges relatively fast.

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 in the future will be performed with robust hybrid optimization algorithms involving automatic switching among constituent optimization algorithms.

ACKNOWLEDGEMENTS

The support provided CNPq, PRH/ANP, CAPES and FAPERJ, Brazilian government agencies for the fostering of science, is greatly appreciated. CNPq support for Prof. Dulikravich to participate in Science Without Borders visit and joint research in Brazil is highly appreciated. This work was also partially funded by the US Air Force Office of Scientific Research under grant FA9550-12-1-0440 monitored by Dr. Ali Sayir. The views and conclusions contained herein are those of the authors and should not be interpreted as necessarily representing the official policies or endorsements, either expressed or implied, of the US Air Force Office of Scientific Research or the U.S. Government. The U.S. Government is authorized to reproduce and distribute reprints for government purposes notwithstanding any copyright notation thereon.

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