GENERALIZED INTEGRAL TRANSFORM TECHNIQUE FOR STURM-LIOUVILLE PROBLEMS IN HETEROGENEOUS MEDIA

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Abstract. *The analytical solution of linear diffusion problems within heterogeneous media requires the computational solution of an eigenvalue problem defined with space variable thermophysical properties. Thus, the GITT is here utilized to handle Sturm-Liouville problems with arbitrarily variable coefficients, by defining eigenfunction expansions in terms of an auxiliary problem of known solution. In addition, the representation of the variable coefficients as eigenfunction expansions themselves, considerably simplifies and accelerates the integral transformation process, by permitting the analytical evaluation of the coefficients matrices that form the transformed algebraic system. The proposed methodology is challenged in solving two different classes of eigenvalue problems in heterogeneous media, as illustrated for the cases of abrupt variations in double layer transitions and of randomly generated distribution functions for the equation coefficients. The convergence behavior of the obtained expansions is then critically inspected and numerical results are presented to offer a set of reference results for eigenvalues and related quantities.*

Keywords*: Heterogeneous media, variable properties, heat conduction, Sturm-Liouville problems, integral transforms*

1. INTRODUCTION

Diffusion problems defined in heterogeneous media involve spatially variable coefficients in different forms, depending on the type of heterogeneity involved, such as large scale variations in functionally graded materials (FGM), abrupt variations in layered composites, and random variations due to local concentration fluctuations in dispersed phase systems, (Lin, 1992), (Qiulin et al., 1999), (Danes et al, 2003). In all such situations, the accurate representation of the diffusion process requires a detailed local solution of the potential behavior, generally with the aid of discrete numerical solutions with sufficient mesh refinement and computational effort and/or semi-analytical approaches for specific or simplified functional forms, as discussed in (Lin, 1992), (Divo & Kassab, 1998), (Fudym et al., 2002), (Sutradhar et al., 2002), (Jiang & Sousa, 2007), (Dai et al., 2007).

Analytical solutions of linear diffusion problems have been analyzed and compiled in (Mikhailov & Ozisik, 1984), where seven different classes of heat and mass diffusion formulations are systematically solved by the classical Integral Transform Method. The obtained formal solutions are applicable over a very broad range of problems in heat and mass transfer, in part illustrated in the referred compendium, including certain examples of diffusion in heterogeneous media. Later on, the classical approach gained a hybrid numerical-analytical implementation and was coined as the Generalized Integral Transform Technique (GITT), (Cotta, 1993), (Cotta & Mikhailov, 1997), (Cotta, 1998), (Cotta & Mikhailov, 2006), offering more flexibility in handling *a priori* non-transformable problems, including, among others, the analysis of nonlinear diffusion and convection-diffusion problems, (Cotta, 1990).

The solution of the associated eigenvalue problem is the major task in the numerical computation of such formal solutions presently available, so as to provide accurate numerical values for the related eigenvalues and normalized eigenfunctions that compose the expansions inherent to the integral transform method. In a number of situations, depending on the specific functional form of the equation coefficients, one may find explicit solutions for the eigenfunctions in terms of special functions which are well documented in textbooks, and more recently, readily available in symbolic computation packages (Wolfram, 2005). On the other hand, for the more general formulation of the eigenvalue problem, a few computational approaches have been developed that offer numerical approximations of the eigenvalues and eigenfunctions, such as the Runge-Kutta method with Pruffer transformation, (Bailey et al., 1978),

(Bailey et al., 1991), the Sign-count method, (Mikhailov & Vulchanov, 1983), (Cotta & Nogueira, 1988), and the GITT itself , (Mikhailov & Cotta, 1994), (Oliveira et al., 1995), (Sphaier & Cotta, 2000).

The GITT has been applied to both the case of variable coefficients (Mikhailov & Cotta, 1994), and irregular domains (Sphaier & Cotta, 2000), and has been recently challenged to handle problems with arbitrary space variations, including large scale and abrupt changes in thermophysical properties due to transition of different materials (Naveira et al., 2008). The approach was first applied in solving an example of spatially variable thermophysical properties found in heat conduction within functionally graded materials (FGM), validated by the exact solution obtained through classical integral transforms in the specific situation of exponentially varying coefficients. Then, the approach is employed for handling a double-layered system with abrupt variation of properties, and critically compared against the exact solution obtained by the classical integral transform method with the adequate discontinuous multi-region eigenvalue problem. The idea is to propose expansions for the desired eigenfunctions themselves, based on an auxiliary problem of known solution. Then, the integral transformation process as applied to the original Sturm-Liouville problem, yields an algebraic transformed system of equations, written as a matrix eigensystem analysis. The numerically computed matrix eigenvalues and eigenvectors allow the reconstruction of the original problem eigenfunctions, which are actually needed in the analytical solution of the proposed diffusion problem.

The present work extends the contribution in (Naveira et al., 2008) and considers the possibility of expressing the variable coefficients themselves as eigenfunction expansions, not necessarily of the same auxiliary eigenvalue problem. This will be particularly advantageous in the evaluation of the algebraic system coefficients matrices, which result from the integration transformation process. All the related integrals can then be expressed in terms of simple eigenfunctions, in general allowing for straightforward analytical evaluations, instead of costly numerical integrations, especially for multidimensional applications. The present methodology can thus be particularly suitable in properties identification tasks and optimization for material properties tailoring. Here, the approach employing the expanded coefficients is challenged to handle the same double-layer abrupt variation situation considered in (Naveira et al., 2008), and then demonstrated for a situation of intense random variation of the equation coefficients along the space variable, such as in (Lin, 1992). After demonstrating the convergence behavior of the related eigenquantities, the random variation case is critically examined against the approximation of effective thermophysical properties values for a range of amplitudes in the maximum variation allowed for.

2. ANALYSIS

We consider a general formulation on transient diffusion for the potential $T(\mathbf{x},t)$, dependent on position $\mathbf{x}$ and time t and defined in region V with boundary surface S. The formulation includes the transient term, the diffusion operator, a linear dissipation term, and an independent source term, (Mikhailov & Ozisik, 1984), Cotta(1993), as shown in problem (1) below. The coefficients $w(\mathbf{x}), k(\mathbf{x}),$ and $d(\mathbf{x})$, are responsible for the information related to the heterogeneity of the medium. The diffusion equation and initial and boundary conditions are given by :

$$w(\mathbf{x})\frac{\partial T(\mathbf{x},t)}{\partial t} = \nabla.[k(\mathbf{x})\nabla T(\mathbf{x},t)] - d(\mathbf{x})T(\mathbf{x},t) + P(\mathbf{x},t), \quad \mathbf{x}\in V, t>0 \tag{1a}$$

$$T(\mathbf{x},0) = f(\mathbf{x}), \quad \mathbf{x}\in V \tag{1b}$$

$$\alpha(\mathbf{x})T(\mathbf{x},t) + \beta(\mathbf{x})k(\mathbf{x})\frac{\partial T(\mathbf{x},t)}{\partial \mathbf{n}} = \phi(\mathbf{x},t), \quad \mathbf{x}\in S \tag{1c}$$

The exact solution of problem (1) is obtained with the Classical Integral Transform Method, (Mikhailov & Ozisik, 1984), and is written as:

$$T(\mathbf{x},t) = \sum_{i=1}^{\infty}\tilde{\psi}_i(\mathbf{x})\left(\overline{f}_i e^{-\mu_i^2 t} + \int_0^t \overline{g}_i(t) e^{-\mu_i^2 (t-t')}dt'\right) \tag{2}$$

where the eigenvalues μ_i and eigenfunctions $\psi_i(\mathbf{x})$, are obtained from the eigenvalue problem that contains the information about the heterogeneous medium, in the form:

$$\nabla.[k(\mathbf{x})\nabla\psi_i(\mathbf{x})] + (\mu_i^2 w(\mathbf{x}) - d(\mathbf{x}))\psi_i(\mathbf{x}) = 0, \quad \mathbf{x}\in V \tag{3a}$$

with boundary conditions

$$\alpha(\mathbf{x})\psi_i(\mathbf{x}) + \beta(\mathbf{x})k(\mathbf{x})\frac{\partial\psi_i(\mathbf{x})}{\partial\mathbf{n}} = 0, \quad \mathbf{x}\in S \tag{3b}$$

Also, the other quantities that appear in the exact solution (2) are computed after solving problem (3), such as:

$$N_i = \int_V w(\mathbf{x})\psi_i^2(\mathbf{x})dv\,, \text{ normalization integrals} \tag{4a}$$

$$\tilde{\psi}_i(\mathbf{x}) = \frac{\psi_i(\mathbf{x})}{\sqrt{N_i}}\,, \text{ normalized eigenfunctions} \tag{4b}$$

$$\overline{f}_i = \int_V w(\mathbf{x})\tilde{\psi}_i(\mathbf{x})f(\mathbf{x})dv\,, \text{ transformed initial condition} \tag{4c}$$

$$\overline{g}_i(t) = \int_V P(\mathbf{x},t)\tilde{\psi}_i(\mathbf{x})dv + \int_S \phi(\mathbf{x},t)[\frac{\tilde{\psi}_i(\mathbf{x}) - k(\mathbf{x})\frac{\partial\tilde{\psi}_i(\mathbf{x})}{\partial\mathbf{n}}}{\alpha(\mathbf{x})+\beta(\mathbf{x})}]ds\,, \text{ transformed source terms} \tag{4d}$$

For a general purpose automatic implementation, it is quite desirable to develop a flexible computational approach to handle eigenvalue problems with arbitrarily variable coefficients, such as problem (3). Thus, the Generalized Integral Transform Technique (GITT) is here employed in the solution of the Sturm-Liouville problem (3) via the proposition of a simpler auxiliary eigenvalue problem, and expanding the unknown eigenfunctions in terms of the chosen basis. Also, the variable equation coefficients are themselves expanded in terms of known eigenfunctions, so as to allow for a fully analytical implementation of the coefficients matrices in the transformed system. The solution of problem (3) is thus proposed as an eigenfunction expansion, in terms of a simpler auxiliary eigenvalue problem, given as:

$$\nabla.[k^*(\mathbf{x})\nabla\Omega_n(\mathbf{x})] + (\lambda_n^2 w^*(\mathbf{x}) - d^*(\mathbf{x}))\Omega_n(\mathbf{x}) = 0,\ \mathbf{x}\in V \tag{5a}$$

with boundary conditions

$$\alpha^*(\mathbf{x})\Omega_n(\mathbf{x}) + \beta^*(\mathbf{x})k^*(\mathbf{x})\frac{\partial\Omega_n(\mathbf{x})}{\partial\mathbf{n}} = 0, \quad \mathbf{x}\in S \tag{5b}$$

where the coefficients $w^*(\mathbf{x}), k^*(\mathbf{x}), and\ d^*(\mathbf{x})$, are simpler forms of the equation coefficients, chosen to allow for an analytical solution of the auxiliary problem. Also, the boundary conditions types of the original and auxiliary problems are allowed to be different, in case further simplification of the auxiliary function is desired, in light of the different boundary condition coefficients, $\alpha^*(\mathbf{x})$ and $\beta^*(\mathbf{x})$.

The proposed expansion of the original expansion is then given by:

$$\psi_i(\mathbf{x}) = \sum_{n=1}^{\infty}\tilde{\Omega}_n(\mathbf{x})\overline{\psi}_{i,n}, \qquad inverse \tag{6a}$$

$$\overline{\psi}_{i,n} = \int_V w^*(\mathbf{x})\psi_i(\mathbf{x})\tilde{\Omega}_n(\mathbf{x})dv, \qquad transform \tag{6b}$$

The integral transformation is thus performed by operating eq.(3a) on with $\int_V \tilde{\Omega}_n(\mathbf{x})-dv$. After employing Green´s 2nd formula so as to account for the difference in boundary conditions of the two eigenvalue problems, it results:

$$\int_V \psi_i(\mathbf{x})(\nabla.[k(\mathbf{x})\nabla\tilde{\Omega}_n(\mathbf{x})])dv + \int_S k(\mathbf{x})(\psi_i(\mathbf{x})\frac{\partial\tilde{\Omega}_n(\mathbf{x})}{\partial\mathbf{n}} - \tilde{\Omega}_n(\mathbf{x})\frac{\partial\psi_i(\mathbf{x})}{\partial\mathbf{n}})ds + \int_V \tilde{\Omega}_n(\mathbf{x})(\mu_i^2 w(\mathbf{x}) - d(\mathbf{x}))\psi_i(\mathbf{x})dv = 0 \tag{7a}$$

Now, by combining boundary conditions (3b) and (5b), the surface integral above can be written as:

$$\int_S k(\mathbf{x})(\psi_i(\mathbf{x})\frac{\partial\tilde{\Omega}_n(\mathbf{x})}{\partial\mathbf{n}} - \tilde{\Omega}_n(\mathbf{x})\frac{\partial\psi_i(\mathbf{x})}{\partial\mathbf{n}})ds = \int_S k(\mathbf{x})(\frac{\alpha(\mathbf{x})}{\beta(\mathbf{x})k(\mathbf{x})} - \frac{\alpha^*(\mathbf{x})}{\beta^*(\mathbf{x})k^*(\mathbf{x})})(\psi_i(\mathbf{x})\tilde{\Omega}_n(\mathbf{x}))ds$$

$$= \int_S k(\mathbf{x})(\frac{\beta^*(\mathbf{x})k^*(\mathbf{x})}{\alpha^*(\mathbf{x})} - \frac{\beta(\mathbf{x})k(\mathbf{x})}{\alpha(\mathbf{x})})(\frac{\partial\psi_i(\mathbf{x})}{\partial\mathbf{n}}\frac{\partial\tilde{\Omega}_n(\mathbf{x})}{\partial\mathbf{n}})ds = -\int_S k(\mathbf{x})(\frac{\beta^*(\mathbf{x})k^*(\mathbf{x})\alpha(\mathbf{x})}{\beta(\mathbf{x})k(\mathbf{x})\alpha^*(\mathbf{x})} - 1)(\psi_i(\mathbf{x})\frac{\partial\tilde{\Omega}_n(\mathbf{x})}{\partial\mathbf{n}})ds \tag{7b}$$

and eq.(7a) can be for instance rewritten as:

$$\int_V \psi_i(\mathbf{x})\nabla.[k(\mathbf{x})\nabla\tilde{\Omega}_n(\mathbf{x})]dv + \int_S k(\mathbf{x})(1-\frac{\beta^*(\mathbf{x})k^*(\mathbf{x})\alpha(\mathbf{x})}{\beta(\mathbf{x})k(\mathbf{x})\alpha^*(\mathbf{x})})(\psi_i(\mathbf{x})\frac{\partial\tilde{\Omega}_n(\mathbf{x})}{\partial\mathbf{n}})ds + \int_V \tilde{\Omega}_n(\mathbf{x})(\mu_i^2 w(\mathbf{x}) - d(\mathbf{x}))\psi_i(\mathbf{x})dv = 0 \tag{7c}$$

Substitution of the inverse formula yields the following algebraic problem:

$$\sum_{m=1}^{\infty}\overline{\psi}_{i,m}(\int_V \tilde{\Omega}_m(\mathbf{x})\nabla.[k(\mathbf{x})\nabla\tilde{\Omega}_n(\mathbf{x})]dv + \int_S k(\mathbf{x})(1-\frac{\beta^*(\mathbf{x})k^*(\mathbf{x})\alpha(\mathbf{x})}{\beta(\mathbf{x})k(\mathbf{x})\alpha^*(\mathbf{x})})(\tilde{\Omega}_m(\mathbf{x})\frac{\partial\tilde{\Omega}_n(\mathbf{x})}{\partial\mathbf{n}})ds + \\ + \int_V \tilde{\Omega}_n(\mathbf{x})(\mu_i^2 w(\mathbf{x}) - d(\mathbf{x}))\tilde{\Omega}_m(\mathbf{x})dv) = 0 \tag{7d}$$

In matrix form, the eigensystem is concisely given by:

$$(\mathbf{A} - \nu\mathbf{B})\overline{\boldsymbol{\psi}} = 0\,, \qquad \text{with} \qquad \nu = \mu^2 \tag{8a}$$

$$\overline{\boldsymbol{\psi}} = \{\overline{\psi}_{n,m}\}; \qquad \mathbf{B} = \{B_{n,m}\}, \quad B_{n,m} = \int_V w(\mathbf{x})\tilde{\Omega}_n(\mathbf{x})\tilde{\Omega}_m(\mathbf{x})dv \tag{8b,c}$$

$$\mathbf{A} = \{A_{n,m}\},$$

$$A_{n,m} = \int_V \tilde{\Omega}_m(\mathbf{x})\nabla.[k(\mathbf{x})\nabla\tilde{\Omega}_n(\mathbf{x})]dv + \int_S k(\mathbf{x})(1-\frac{\beta^*(\mathbf{x})k^*(\mathbf{x})\alpha(\mathbf{x})}{\beta(\mathbf{x})k(\mathbf{x})\alpha^*(\mathbf{x})})(\tilde{\Omega}_m(\mathbf{x})\frac{\partial\tilde{\Omega}_n(\mathbf{x})}{\partial\mathbf{n}}ds - \int_V d(\mathbf{x})\tilde{\Omega}_n(\mathbf{x})\tilde{\Omega}_m(\mathbf{x})dv \tag{8d}$$

Also, accounting for the auxiliary problem formulation, the system matrix **A** can be rewritten as:

$$A_{n,m} = \int_V \tilde{\Omega}_m(\mathbf{x})\nabla.[(k(\mathbf{x}) - k^*(\mathbf{x}))\nabla\tilde{\Omega}_n(\mathbf{x})]dv + \int_S (k(\mathbf{x}) - \frac{\beta^*(\mathbf{x})\alpha(\mathbf{x})}{\beta(\mathbf{x})\alpha^*(\mathbf{x})}k^*(\mathbf{x}))(\tilde{\Omega}_m(\mathbf{x})\frac{\partial\tilde{\Omega}_n(\mathbf{x})}{\partial\mathbf{n}})ds - \\ -\int_V (d(\mathbf{x}) - d^*(\mathbf{x}))\tilde{\Omega}_n(\mathbf{x})\tilde{\Omega}_m(\mathbf{x})dv + \lambda_n^2\delta_{n,m} \tag{8d}$$

The algebraic problem (8) can be numerically solved to provide results for the eigenvalues and eigenvectors, which will be combined by the inverse formula (6a) to provide the desired eigenfunctions.

It is also relevant to consider the possibility of expressing the variable coefficients themselves as eigenfunction expansions, in general not of the same auxiliary eigenvalue problem. This is particularly advantageous in the evaluation of the algebraic system coefficients, $A_{n,m}$ and $B_{n,m}$. All the related integrals can then be expressed in terms of eigenfunctions, in general allowing for straightforward analytical evaluations. For instance, the coefficient $w(\mathbf{x})$ can be expanded in terms of eigenfunctions, together with a filtering solution to enhance convergence, in the following form:

$$w(\mathbf{x}) = w_f(\mathbf{x}) + \sum_{k=1}^{\infty}\tilde{\Gamma}_k(\mathbf{x})\overline{w}_k, \qquad \textit{inverse} \tag{9a}$$

$$\overline{w}_k = \int_V \hat{w}(\mathbf{x})[w(\mathbf{x}) - w_f(\mathbf{x})]\tilde{\Gamma}_k(\mathbf{x})d\mathbf{x}, \qquad \textit{transform} \tag{9b}$$

where $\hat{w}(\mathbf{x})$ is the weighting function for the chosen normalized eigenfunction $\tilde{\Gamma}_k(\mathbf{x})$. For instance, the eigenfunction basis may be chosen employing the same auxiliary problem equation, but with first order boundary conditions throughout, while the filtering function would be a simple analytic function that satisfies the boundary values for the original coefficients. Then, once the transformed coefficients have been obtained through the transform formula, eq.(9b), computations may be carried on with the inverse expression for the variable coefficient, eq.(9a). This procedure might also be of interest in function estimation tasks, when the transformed quantities would be the parameters to be estimated. The two remaining coefficients are equally expanded, if necessary, in terms of eigenfunctions, here assumed to be equal just for the sake of conciseness, to yield:

$$k(\mathbf{x}) = k_f(\mathbf{x}) + \sum_{k=1}^{\infty}\tilde{\Gamma}_k(\mathbf{x})\overline{k}_k, \qquad \textit{inverse} \tag{10a}$$

$$\bar{k}_k = \int_V \hat{w}(\mathbf{x})[k(\mathbf{x}) - k_f(\mathbf{x})]\tilde{\Gamma}_k(\mathbf{x})d\mathbf{x}, \qquad transform \tag{10b}$$

$$d(\mathbf{x}) = d_f(\mathbf{x}) + \sum_{k=1}^{\infty} \tilde{\Gamma}_k(\mathbf{x})\bar{d}_k, \qquad inverse \tag{11a}$$

$$\bar{d}_k = \int_V \hat{w}(\mathbf{x})[d(\mathbf{x}) - d_f(\mathbf{x})]\tilde{\Gamma}_k(\mathbf{x})d\mathbf{x}, \qquad transform \tag{11b}$$

The matrices coefficients may then be rewritten in terms of the expanded functions, such as for the elements of matrix **B**:

$$B_{n,m} = \int_V w_f(\mathbf{x})\tilde{\Omega}_n(\mathbf{x})\tilde{\Omega}_m(\mathbf{x})dv + \sum_{k=1}^{\infty} \bar{w}_k \int_V \tilde{\Gamma}_k(\mathbf{x})\tilde{\Omega}_n(\mathbf{x})\tilde{\Omega}_m(\mathbf{x})dv \tag{12a}$$

and for matrix **A**:

$$A_{n,m} = \int_V \tilde{\Omega}_m(\mathbf{x})\nabla.[(k_f(\mathbf{x}) - k^*(\mathbf{x}))\nabla\tilde{\Omega}_n(\mathbf{x})]dv + \sum_{k=1}^{\infty}[\int_V \tilde{\Omega}_m(\mathbf{x})\nabla.[\tilde{\Gamma}_k(\mathbf{x})\nabla\tilde{\Omega}_n(\mathbf{x})]dv]\bar{k}_k +$$

$$+\int_S [k_f(\mathbf{x}) - \frac{\beta^*(\mathbf{x})\alpha(\mathbf{x})}{\beta(\mathbf{x})\alpha^*(\mathbf{x})}k^*(\mathbf{x})](\tilde{\Omega}_m(\mathbf{x})\frac{\partial\tilde{\Omega}_n(\mathbf{x})}{\partial\mathbf{n}})ds + \sum_{k=1}^{\infty}[\int_S \tilde{\Gamma}_k(\mathbf{x})(\tilde{\Omega}_m(\mathbf{x})\frac{\partial\tilde{\Omega}_n(\mathbf{x})}{\partial\mathbf{n}})ds]\bar{k}_k - \tag{12b}$$

$$-\int_V (d_f(\mathbf{x}) - d^*(\mathbf{x}))\tilde{\Omega}_n(\mathbf{x})\tilde{\Omega}_m(\mathbf{x})dv - \sum_{k=1}^{\infty}[\int_V \tilde{\Gamma}_k(\mathbf{x})\tilde{\Omega}_n(\mathbf{x})\tilde{\Omega}_m(\mathbf{x})dv]\bar{d}_k + \lambda_n^2\delta_{n,m}$$

The norms are then computed from:

$$N_i = \sum_{n=1}^{\infty}\sum_{m=1}^{\infty}\bar{\psi}_{i,n}\bar{\psi}_{i,m}\{\int_V w_f(\mathbf{x})\tilde{\Omega}_n(\mathbf{x})\tilde{\Omega}_m(\mathbf{x})dv + \sum_{k=1}^{\infty}[\int_V \tilde{\Gamma}_k(\mathbf{x})\tilde{\Omega}_n(\mathbf{x})\tilde{\Omega}_m(\mathbf{x})dv]\bar{w}_k\} \tag{13}$$

3. APPLICATIONS

The problems here considered involve the analysis of two quite different situations, one related with an abrupt variation of thermophysical properties, typical of the transition between two materials layers (Orlande et al., 2008), and the second associated with random variation of the thermophysical properties, (Lin, 1992). The problem formulation in both cases is given by:

$$w(x)\frac{\partial T(x,t)}{\partial t} = \frac{\partial}{\partial x}[k(x)\frac{\partial T(x,t)}{\partial x}], \quad 0 < x < 1, \quad t > 0 \tag{14a}$$

with initial and boundary conditions

$$T(x,0) = f(x), \quad 0 < x < 1 \tag{14b}$$

$$\left.\frac{\partial T(x,t)}{\partial x}\right|_{x=0} = 0, \qquad \left.\frac{\partial T(x,t)}{\partial x}\right|_{x=1} = 0, \quad t > 0 \tag{14c,d}$$

The initial condition is arbitrarily chosen as $f(x)=1-x^2$ for the present illustration. The space variable coefficients for the abrupt variation are governed by the parameter γ in the function below

$$k(x) = k_1 + (k_2 - k_1)\delta(x), \qquad w(x) = w_1 + (w_2 - w_1)\delta(x) \tag{15a,b}$$

$$\delta(x) = \frac{1}{1 + e^{-\gamma(x - xc)}} \tag{15c}$$

with x_c being the interface position.

The randomly generated coefficients were obtained based on the example of (Lin, 1992), by first generating a number of positions within the medium, and then producing random scaling factors for the properties variations at each position, normalized by their average value. The resulting values are then interpolated to provide continuous functions. A gain parameter is also defined to allow for an inspection of the accuracy of effective thermophysical properties in simplifying the problem formulation, as shall be discussed in the results and discussion section. The variable coefficients are the given by:

$$k(x) = k_0\left[1+\left(\frac{g_1(x)}{\bar{g}_1}-1\right)G\right], \qquad w(x) = w_0\left[1+\left(\frac{g_2(x)}{\bar{g}_2}-1\right)G\right] \tag{16a,b}$$

where $g_1(x)$ and $g_2(x)$ are the linearly interpolated functions of the properties values, randomly generated in the interval [0,1] within selected positions x, and $\bar{g}_1$ and $\bar{g}_2$ are the corresponding average values of these two functions. The constant factor G reflects the extent of the effects of random numbers on the two thermal properties functions $k(x)$ and $w(x)$. For instance, with G=1 one obtains the full random pattern of the generated functions, while G=0 recovers the uniform thermophysical properties situation. The eigenvalue problem to be solved is then given by:

$$\frac{d}{dx}[k(x)\frac{d\psi_i(x)}{dx}]+\mu_i^2 w(x)\psi_i(x)=0, \qquad 0<x<1 \tag{17a}$$

with boundary conditions

$$\left.\frac{d\psi_i(x)}{dx}\right|_{x=0}=0, \qquad \left.\frac{d\psi_i(x)}{dx}\right|_{x=1}=0 \tag{17b,c}$$

So as to demonstrate the potential applicability of the present approach, the simplest possible auxiliary problem was considered, based on the choice of coefficients $k^*(x)$=1, $w^*(x)$=1, and $d^*(x)$=0, and maintaining the same boundary conditions as in eqs.(17b,c), which results in:

$$\tilde{\Omega}_n(x)=\sqrt{2}\,cos(\lambda_n x), \quad \text{and} \quad \tilde{\Omega}_0(x)=1, \quad \text{with} \quad \lambda_n=n\pi, \quad n=0,1,2... \tag{18a-c}$$

4. RESULTS AND DISCUSSION

Before proceeding to the solution of the Sturm-Liouville problem for such heterogeneous media examples, we illustrate the convergence of the eigenfunction expansion representations of the variable coefficients themselves, in each case. For instance, Figures 1.a,b illustrate the behavior of the variable coefficient $k(x)$ for the double-layer example, together with its eigenfunction expansion, with k_1=1, k_2=20, x_c=0.3, and for different values of the parameter γ = 20 and 200. To the graph scale, the value γ=200 produces a practically vertical variation on the thermophysical properties. We have chosen to adopt as a filter the straight line that connects the two extreme values, $k(0)$ and $k(1)$, not accounting for the knowledge of the interface position. The eigenfunction was taken from the same auxiliary problem equation, but with first kind boundary conditions, i.e.:

$$\tilde{\Gamma}_k(x)=\sqrt{2}\,sin(\nu_k x), \quad \text{with} \quad \nu_k=k\pi, \quad k=1,2,3... \tag{18a-c}$$

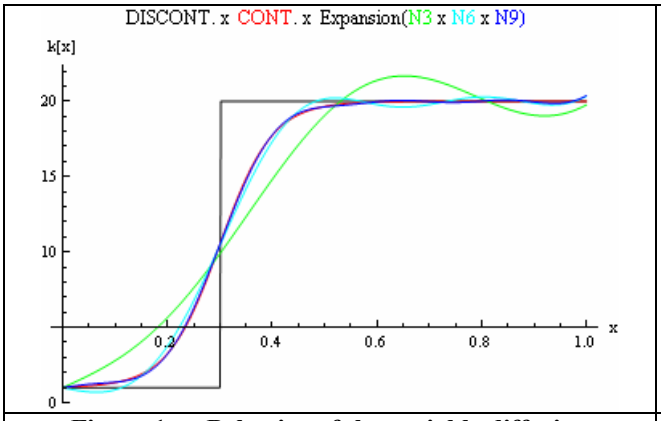

Figure 1.a– Behavior of the variable diffusion coefficient *k(x)* and its eigenfunction expansion for the double-layer example, with γ=20 and truncation orders N=3, 6, and 9.

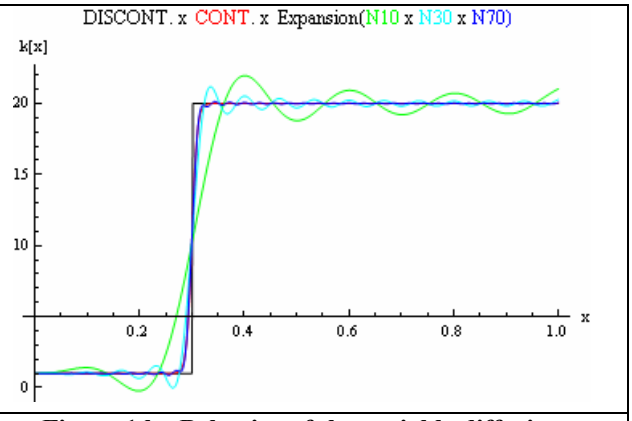

Figure 1.b– Behavior of the variable diffusion coefficient *k(x)* and its eigenfunction expansion for the double-layer example, with γ=200 and truncation orders N=10, 30, and 70.

For the case with the less abrupt space variation, Fig.1.a, convergence of the coefficient expansion is achieved to the graph scale with very low truncation orders, such as N=9 (dark blue) which overwrites the red curve for the original coefficient, eq.(15a) .For the case of an actual abrupt variation, Fig.1.b, a larger number of terms were required for the expansion to appropriately recover the coefficient behavior, as illustrated by the curve with N=70, which is

practically coincident with the continuous curve in red which is not visible, being overwritten by the dark blue curve (N=70).

Similar results were obtained and analyzed for the random properties example, as illustrated below in Figures 2.a,b for the *k(x)* coefficient by taking k_0=0.5, with *G*=0.2 and 0.8. A total of 40 equally spaced points were taken along the domain for the random properties generation, while the random numbers at each position were kept unchanged for the two cases of different gains. The truncation orders for the coefficient expansion are illustrated for N=20, 40, and 80. Clearly, the case with the smaller gain, G=0.2, presents a better convergence behavior, due to the dumping effect on the oscillations amplitudes, with the results for N= 80 being fully coincident with the interpolated original curves in black that are overwritten by the red curve (N=80). For the case with larger amplitudes in the random variations, G=0.8, the curve for N=40 still presents noticeable deviations from the original interpolated curve, while the red curve for N=80 practically overwrites the original coefficient in black, except at the very sharp edges which would still require a few extra terms. The same trends were observed for the randomly generated *w(x)* behavior, generated for w_0=0.5 and also for 40 equally spaced points, as illustrated in Figures 3.a,b below. As opposed to the case in (Lin, 1992), the two coefficients were allowed to be independently generated, to further challenge the proposed approach.

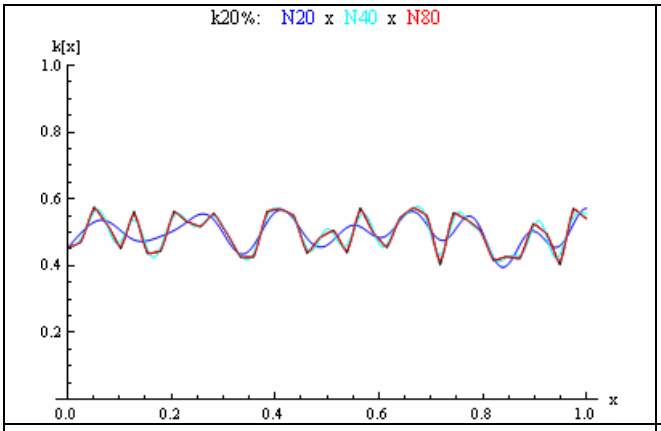

Figure 2.a– Behavior of the variable diffusion coefficient *k(x)* and its eigenfunction expansion for the random properties example, with *G*=0.2 and truncation orders N=20, 40, and 80.

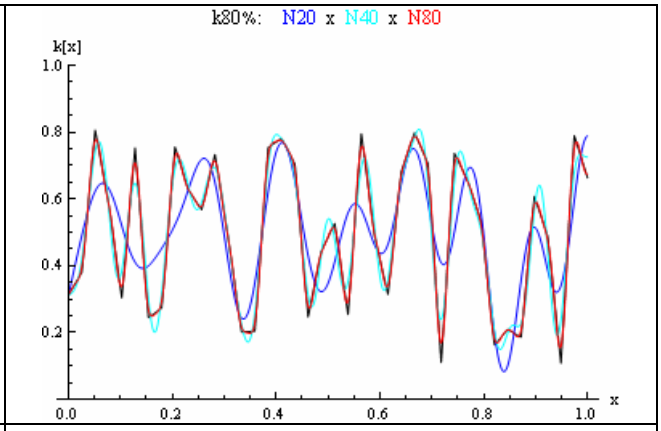

Figure 2.b– Behavior of the variable diffusion coefficient *k(x)* and its eigenfunction expansion for the random properties example, with *G*=0.8 and truncation orders N=20, 40, and 80.

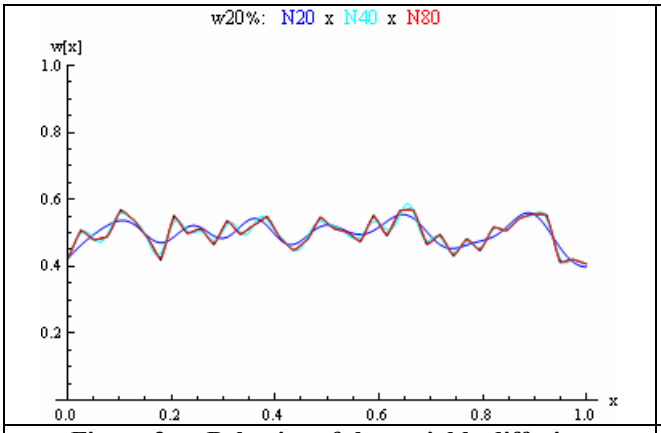

Figure 3.a– Behavior of the variable diffusion coefficient w*(x)* and its eigenfunction expansion for the random properties example, with *G*=0.2 and truncation orders N=20, 40, and 80.

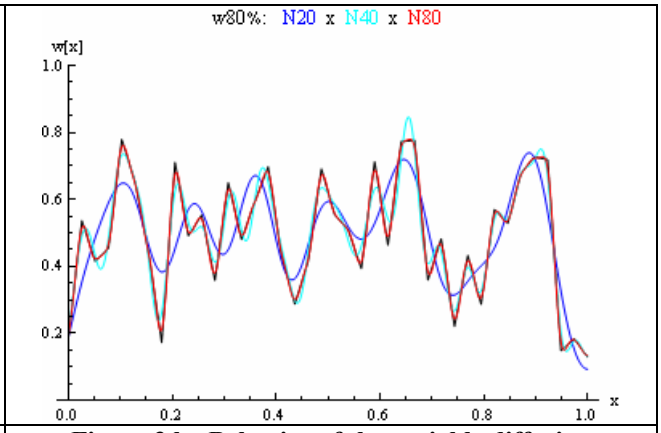

Figure 3.b– Behavior of the variable diffusion coefficient w*(x)* and its eigenfunction expansion for the random properties example, with *G*=0.8 and truncation orders N=20, 40, and 80.

The eigenvalue problem solution is now demonstrated, first by considering the double-layer example, again with k_1=1, k_2=20, x_c=0.3, w_1=1 and w_2=4, with γ=20 and 200. Tables 1.a,b then show the converged values of the first ten eigenvalues μ_i´s for different truncation orders in the coefficients expansions, N, compared in the last two columns with the original continuous function behavior and the exact discontinuous eigenvalue problem solution, here shown just as a limiting case (Naveira et al., 2008). The eigenfunction expansions were fixed to truncation orders M=50 in the case of γ=20, and M=100 for γ=200, which are more than sufficient to provide converged results to the first ten eigenvalues here presented, as achieved for the original coefficients representation in (Naveira et al., 2008). In Table 1.a, for the smoother coefficients behavior, fairly low truncation orders (N=27) in the coefficients expansions already

provides four significant digits of convergence in the first ten eigenvalues, as compared to the eigenvalues obtained with the numerical integration based on the original coefficients representations. On the other hand, for the very abrupt variation case, for γ=200, it is shown in Table 1.b that N=90 terms are required to yield four fully converged significant digits in these same first ten eigenvalues. It is also evident that the results in Table 1.b are now much closer to the exact solution of the discontinuous case (Naveira et al., 2008), as the coefficients representation approach constant values in each layer.

Table 1.a – Influence of the coefficients expansion order on the eigenvalues for double-layer problem and γ=20.

Order i	N=3	N=9	N=15	N=21	N=27	Original Coefficients	Discontinuous Problem
1	7.86217	7.55814	7.58512	7.58441	7.58398	7.58283	5.21316
2	12.8587	11.0763	11.1109	11.1094	11.1088	11.1073	10.0779
3	18.8689	18.1683	18.1250	18.1222	18.1209	18.1192	15.6389
4	24.9545	23.6561	23.4347	23.4324	23.4276	23.4233	20.1568
5	31.0633	29.2863	29.1625	29.1714	29.1646	29.1589	26.0627
6	37.1900	35.0534	34.9998	35.0180	35.0151	35.0040	30.238
7	43.3268	40.8122	40.6868	40.6945	40.7094	40.6934	36.4832
8	49.4702	46.5966	46.4962	46.4989	46.5245	46.5102	40.3228
9	55.6181	52.3889	52.2518	52.2658	52.2762	52.2744	46.8986
10	61.7694	58.1812	58.0240	58.0518	58.0539	58.0618	50.4129

Table 1.b – Influence of the coefficients expansion order on the eigenvalues for double-layer problem and γ=200.

Order i	N=10	N=30	N=50	N=70	N=90	Original Coefficients	Discontinuous Problem
1	6.46777	3.84373	5.35180	5.43558	5.44368	5.44376	5.21316
2	9.35032	10.0036	10.0759	10.0800	10.0805	10.0805	10.0779
3	11.9257	13.4899	16.0827	16.2949	16.3144	16.3139	15.6389
4	17.1314	19.9054	20.1559	20.1772	20.1793	20.1794	20.1568
5	20.0420	24.4230	26.7905	27.1017	27.1296	27.1284	26.0627
6	26.0591	29.7795	30.2563	30.3164	30.3214	30.3213	30.238
7	30.3240	35.8098	37.4216	37.8060	37.8413	37.8402	36.4832
8	36.1541	39.6127	40.3890	40.5337	40.5439	40.5431	40.3228
9	40.9689	49.2159	47.9487	48.3579	48.3992	48.3994	46.8986
10	46.6208	50.6779	50.5490	50.8692	50.8904	50.8882	50.4129

Now, the random properties case is more closely examined, initiating by the illustration of the convergence behavior of the first ten eigenvalues for a fixed order in the coefficients expansion (N=60) but with increasing order in the eigenfunction expansion (M<150). The aim is to demonstrate that the proposed approach is capable of reaching convergence on the eigenvalues of such a variable coefficients behavior for the worst case of G=1, to within reasonable values of the expansion orders. As can be observed in Table 2 below, at least four significant digits are fully converged within the first ten eigenvalues, in the present range of truncation orders for the original problem eigenfunction expansion (M).

Table 2 – Convergence of the first ten eigenvalues for random properties case, with G=1 and *N*=60.

Order i	M=30	M=50	M=70	M=90	M=110	M=130	M=150
1	2.90207	2.81610	2.79202	2.78723	2.78543	2.78468	2.78438
2	5.23384	5.10513	5.03219	5.02071	5.01469	5.01261	5.01180
3	8.10109	7.98097	7.92827	7.92255	7.92061	7.92003	7.91992
4	11.0147	10.7324	10.6851	10.6721	10.6689	10.6669	10.6664
5	14.2049	13.7071	13.5311	13.4519	13.4224	13.4082	13.4039
6	18.0462	17.5109	17.4131	17.3517	17.3373	17.3297	17.3277
7	21.7980	21.3897	21.3193	21.2939	21.2905	21.2893	21.2889
8	23.8627	22.7361	22.5215	22.3882	22.3555	22.3438	22.3379
9	26.1779	25.4687	25.2890	25.2408	25.2231	25.2162	25.2133
10	28.0186	27.1276	26.9681	26.9264	26.9131	26.9092	26.9077

In addition, the influence of the coefficients expansions truncation orders (N) on the behavior of the eigenvalues of problem (17) is investigated, for the selected truncation orders, N=20, 40, 60, and 80, and the coefficients given as in Figs. 2.a,b and 3.a,b, respectively for G=0.2 and 0.8. The fully converged first ten eigenvalues are shown for the four truncation orders, while the last column stands for the exact solution of the constant properties case taking the average values (k_0=0.5, w_0=0.5), which corresponds to letting G=0 ($\mu_i=i\pi$). One may see that the case

G=0.2 (Table 3.a) presents a faster convergence behavior, with five significant digits fully converged at N=80, and four digits even at much lower orders (N=40). The case G=0.8 (Table 3.b) requires N=80 for convergence to three or four digits Also, the case G=0.2 in much closer to the average coefficients case than the case of larger amplitudes (G=0.8).

Table 3.a – Influence of the coefficients expansion order on the eigenvalues convergence for random properties case, with *G*=0.2 and M=130.

Order i	N=20	N=40	N=60	N=80	Average Coefficients
1	3.16449	3.15729	3.15689	3.15686	3.14159
2	6.28282	6.26935	6.26850	6.26838	6.28319
3	9.35681	9.33976	9.33878	9.33878	9.42478
4	12.6530	12.6170	12.6161	12.6160	12.5664
5	15.7713	15.7373	15.7349	15.7347	15.7080
6	19.0701	19.0190	19.0164	19.0160	18.8496
7	22.2023	22.1164	22.1171	22.1168	21.9911
8	24.9620	24.8902	24.8873	24.8868	25.1327
9	28.0636	27.9403	27.9376	27.9368	28.2743
10	31.4196	31.0352	31.0298	31.0296	31.4159

Table 3.b – Influence of the coefficients expansion order on the eigenvalues convergence for random properties case, with *G*=0.8 and M=130.

Order i	N=20	N=40	N=60	N=80	Average Coefficients
1	3.06151	2.99641	2.98972	2.98923	3.14159
2	5.62010	5.67426	5.65784	5.65421	6.28319
3	8.55875	8.50327	8.50833	8.51195	9.42478
4	12.1256	11.6373	11.6541	11.6590	12.5664
5	15.1172	14.8270	14.6997	14.6918	15.7080
6	19.0776	18.4934	18.3607	18.3456	18.8496
7	22.8903	21.7319	21.7461	21.7476	21.9911
8	24.0256	23.9314	23.9213	23.8994	25.1327
9	27.4253	26.3126	26.2995	26.2807	28.2743
10	31.2083	28.4118	28.4003	28.4079	31.4159

Finally, we examine the behavior of the temperature distribution within the medium, as a function of the gain G for the values G=0, 0.2, 0.5, 0.8 and 1, which governs the amplitude of the coefficients variations, but maintaining the same random numbers at each *x* for the different gains. Figures 4.a,b illustrate the temperature profile behavior at two different dimensionless times, respectively, for t=0.05 and 0.1. The base case G=0 provides the result for the constant properties situation, when the properties local variations are ignored and substituted by an effective average value. As we can see, the differences between the variable and constant coefficients cases are more significant for increasing G and time value, and closer to the boundary x=1 for this particular application. A reasonable reproduction of the actual heterogeneous problem solution when employing effective values, is achieved only for the moderate case of G=0.2.

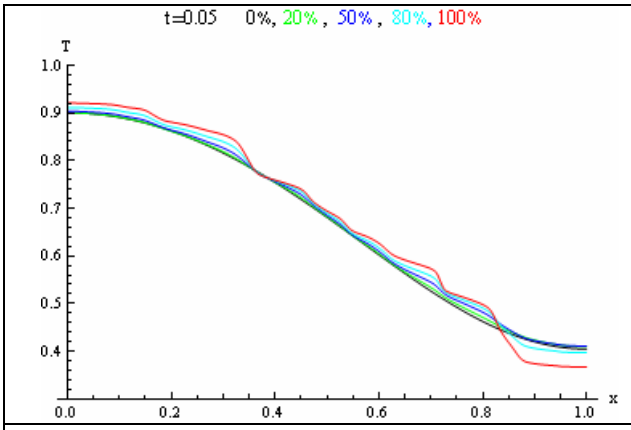

Figure 4.a– Temperature distribution for the random properties example at t=0.05, with *G*=0, 0.2, 0.5, 0.8 and 1, and truncation orders M=130 and N=80.

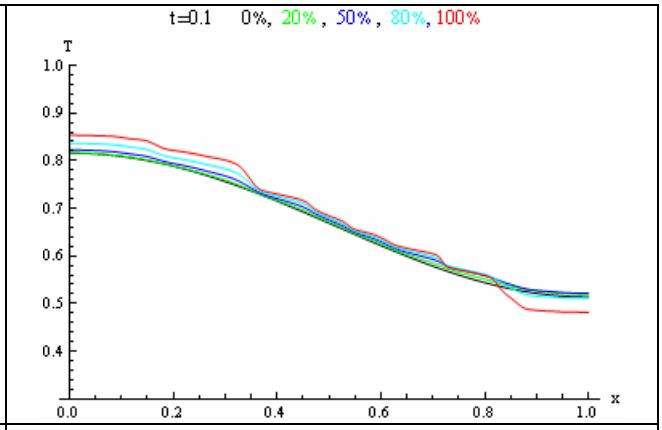

Figure 4.b–Temperature distribution for the random properties example at t=0.1, with *G*=0, 0.2, 0.5, 0.8 and 1, and truncation orders M=130 and N=80.

5. ACKNOWLEDGEMENTS

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