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IMPROVED EIGENFUNCTION EXPANSIONS IN DIFFUSION PROBLEMS WITH MULTISCALE SPACE VARIABLE COEFFICIENTS

RenatoMachado Cotta, cotta@mecanica.coppe.ufrj.br
Universidade Federal do Rio de Janeiro, DEM/PEM. POLI &COPPE/UFRJ

Carolina Palma Naveira-Cotta, carolina@mecanica.coppe.ufrj.br
Universidade Federal do Rio de Janeiro, DEM/PEM. POLI &COPPE/UFRJ

Diego Campos Knupp, diegoknupp@iprj.uerj.br
Instituto Politécnico, Universidade do Estado do Rio de Janeiro, IPRJ/UERJ

Abstract. *The Generalized Integral Transform Technique (GITT) is described for solving diffusion problems defined in physical domains with subregions of multiple materials and/or spatial scales. Recently, through a single domain reformulation strategy, multiregion problems have been reformulated as a single domain with space variable coefficients, in which the subregions transitions are incorporated into one single eigenvalue problem for the proposed eigenfunction expansions. Then, the eigenfunctions spatial behaviors are responsible for recovering the local information in each subregion, thus avoiding cumbersome domain decomposition schemes, while the transformed ordinary differential equations system handles the temporal behavior of the solution. The GITT itself can be employed in the solution of the corresponding eigenvalue problem with space variable coefficients, by adopting a simpler auxiliary eigenvalue problem for the eigenfunction representation in each space coordinate, resulting in a matrix eigenvalue problem that is readily solved for. An integral balance approach to improve the convergence behavior of the eigenfunction expansions, while offering explicit accounting for the space variable coefficients, is then here proposed. An example is provided that deals with heat conduction in heterogeneous media, such as in functionally graded materials, with multiscale variation of thermophysical properties across the domain. The convergence characteristics of the integral transforms solution is more closely examined and critically compared against fully converged results from the available exact solution.*

Keywords: *Conduction Heat Transfer, Eigenfunction Expansions, Integral Transforms, Heterogeneous Media, GITT*

1. INTRODUCTION

A number of applications in heat and fluid flow offers challenging mathematical formulations in convection-diffusion with abrupt and/or multiscale spatial variations in the associated linear or nonlinear partial differential equations coefficients. These governing parameters behavior may originate, for instance, from natural or tailored physical properties variability in heterogeneous media and from abrupt material transitions in multiregion geometries such as in multilayered media or conjugated problems [1-6].

A few different approaches have been proposed to effectively deal with such spatial variations throughout computational domains [3-11], including some attempts of benefiting from semi-analytical solution implementations, towards more robust and cost-effective simulations to be employed in combination with computationally intensive tasks, such as optimization, inverse problem analysis, and simulation under uncertainty.

One such hybrid numerical-analytical approach, known as the Generalized Integral Transform Technique [12-17], as briefly reviewed above, has been employed in the solution of diffusion problems in heterogeneous media with abrupt and multiscale spatial variations in thermophysical properties [3-6]. Originally in connection with conjugated heat transfer problems [5-6], a reformulation strategy coined as the single domain approach has been introduced to rewrite a multiregion problem into one single region with space variable thermophysical properties and source terms, so as to allow for a single integral transformation of the whole domain. This strategy is quite convenient in dealing with complex configurations and irregular regions as well, as recently illustrated [5-6], and has a potential for further extension aiming at automatic implementations of the integral transform procedure, as recently achieved through the so called UNIT (Unified Integral Transforms) algorithm [18-21].

In any such cases, the resulting convection-diffusion equations with space variable coefficients, for each associated potential, can be solved through integral transforms by adopting eigenvalue problems that carry the information on the variable coefficients. The eigenvalue problems are themselves handled by the GITT [13, 22-23], transforming the differential eigenvalue problems into algebraic eigensystems which can be handled very efficiently by widely available subroutines and computational platforms [24]. It has been observed in these recent developments that the eigenfunction expansions of such eigenvalue problems can experience a slower convergence rate for abrupt and/or multiscale variations on the governing coefficients. Therefore, it becomes of interest to propose a convergence enhancement technique to allow for computational savings and accuracy improvement on the GITT application in such cases.

Thus, based on previous developments on convergence enhancement of eigenfunction expansions for diffusion problems [25-26], by employing an integral balance analytical procedure, the GITT solution of eigenvalue problems is here revisited so as to provide accelerated eigenfunctions convergence, explicitly accounting for the space variable coefficients of the original problem formulation, within the resulting functional form of the redefined inverse formulae for the eigenfunctions. Working expressions are provided for a general one-dimensional Sturm-Liouville problem, and the approach is tested for a FGM (functionally graded material) heat conduction problem with a multiscale space variation of thermophysical properties.

2. FORMAL SOLUTION

We consider the nonlinear convection-diffusion problem below

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

subjected to the following initial and boundary conditions:

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

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

The proposed problem is more general than it seems at first glance, since any type of nonlinearities in the equation and boundary condition coefficients can be moved to the corresponding source terms, $P(\mathbf{x},t,T)$ and $\phi(\mathbf{x},t,T)$, without loss of generality. In this sense, the linear equation (w, k, d) and boundary condition (α, β) coefficients are essentially characteristic expressions that are chosen so as to intrinsically formulate the eigenvalue problem that shall be adopted as a basis for the eigenfunction expansion solution that shall follow.

However, before applying the integral transforms solution methodology, it is recommended to reduce the importance of the source terms in the original equation and the boundary conditions given by Eqs. (1a,c), since these are essentially responsible for an eventual slower convergence behavior, by applying a filtering scheme, such as in the general form given by:

$$T(\mathbf{x},t)=T^*(\mathbf{x},t)+T_F(\mathbf{x},t,T^*) \tag{2}$$

where $T_F(\mathbf{x},t,T^*)$ is the proposed known filter and $T^*(\mathbf{x},t)$ is the resulting filtered potential to be determined. After introducing Eq. (2) into Eqs. (1), it results

$$w(\mathbf{x})\frac{\partial T^*(\mathbf{x},t)}{\partial t}=\nabla\cdot[k(\mathbf{x})\nabla T^*(\mathbf{x},t)]-d(\mathbf{x})T^*(\mathbf{x},t)+P^*(\mathbf{x},t,T^*),\quad \mathbf{x}\in V,\ t>0 \tag{3a}$$

$$T^*(\mathbf{x},0)=f^*(\mathbf{x}),\quad \mathbf{x}\in V \tag{3b}$$

$$\alpha(\mathbf{x})T^*(\mathbf{x},t)+\beta(\mathbf{x})k(\mathbf{x})\frac{\partial T^*(\mathbf{x},t)}{\partial \mathbf{n}}=\phi^*(\mathbf{x},t,T^*),\quad \mathbf{x}\in S \tag{3c}$$

where

$$f^*(\mathbf{x})\equiv f(\mathbf{x})-T_F(\mathbf{x},0,f^*(\mathbf{x})) \tag{4.a}$$

$$P^*(\mathbf{x},t,T^*)=P(\mathbf{x},t,T)-w(\mathbf{x})\frac{\partial T_F(\mathbf{x},t,T^*)}{\partial t}+\nabla\cdot[k(\mathbf{x})\nabla T_F(\mathbf{x},t,T^*)]-d(\mathbf{x})T_F(\mathbf{x},t,T^*) \tag{4.b}$$

$$\phi^*(\mathbf{x},t,T^*)=\phi(\mathbf{x},t,T)-\alpha(\mathbf{x})T_F(\mathbf{x},t,T^*)-\beta(\mathbf{x})k(\mathbf{x})\frac{\partial T_F(\mathbf{x},t,T^*)}{\partial \mathbf{n}},\quad \mathbf{x}\in S \tag{4.c}$$

As from Eq.(2), either a linear explicit filter, $T_F(\mathbf{x},t)$, or a nonlinear implicit filter, $T_F(\mathbf{x},t,T)$, can be chosen, with the inherently more simple expressions, in the choice of a linear filter, for the filtered initial conditions and source terms obtained from Eqs. (4). In any case, it is in general desirable that the chosen filter at least satisfies Eq.(1.c), so as to homogenize the boundary conditions, thus leading to $\phi^*(\mathbf{x},t,T^*)=0$.

Following the steps in the integral transform approach [12-17], we define an auxiliary eigenvalue problem, which shall provide the basis for the eigenfunction expansions, in the form

$$\nabla\cdot[k(\mathbf{x})\nabla\psi_i(\mathbf{x})]+[\mu_i^2 w(\mathbf{x})-d(\mathbf{x})]\psi_i(\mathbf{x})=0,\quad \mathbf{x}\in V \tag{5.a}$$

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

The eigenvalue problem given by Eqs. (5) allows for the definition of the integral transform pair below:

$$\bar{T}_i(t) = \int_V w(\mathbf{x})\psi_i(\mathbf{x})T^*(\mathbf{x},t)dV \text{ , } \quad \text{transform} \tag{6.a}$$

$$T^*(\mathbf{x},t) = \sum_{i=1}^{\infty} \frac{1}{N_i} \psi_i(\mathbf{x})\bar{T}_i(t) \text{ , } \quad \text{inverse} \tag{6.b}$$

and the normalization integral

$$N_i = \int_v w(\mathbf{x})\psi_i^2(\mathbf{x})\, dV \tag{7}$$

After application of the integral transformation procedure, through the operator $\int_v \psi_i(\mathbf{x})\,(.)\,dV$ over Eq.(3.a), and $\int_v w(\mathbf{x})\psi_i(\mathbf{x})\,(.)\,dV$ over Eq.(3.b), the resulting ODE system for the transformed potentials, $\bar{T}_i(t)$, is written as:

$$\frac{d\bar{T}_i(t)}{dt} + \mu_i^2\, \bar{T}_i(t) = \bar{g}_i(t,\bar{\mathbf{T}}), \text{ t> 0, } \quad \text{i, j = 1,2…} \tag{8.a}$$

with initial conditions

$$\bar{T}_i(0)=\bar{f}_i \tag{8.b}$$

where,

$$\bar{g}_i(t,\bar{\mathbf{T}}) = \int_v \psi_i(\mathbf{x})P^*(\mathbf{x},t,T^*)\, dV + \int_S \phi^*(\mathbf{x},t,T^*) \left(\frac{\psi_i(\mathbf{x}) \; - k(\mathbf{x})\frac{\partial \psi_i}{\partial \mathbf{n}}}{\alpha(\mathbf{x}) + \beta(\mathbf{x})} \right) dS \tag{8.c}$$

$$\bar{f}_i = \int_v w(\mathbf{x})\; \tilde{\psi}_i(\mathbf{x})\, f^*(\mathbf{x})\; \mathrm{d}V \tag{8.d}$$

$$\bar{\mathbf{T}} = \left\{ \bar{T}_1(t), \bar{T}_2(t), \ldots \right\}^T \tag{8.e}$$

System (8) is then numerically solved through well-established initial value problem solvers, readily available in scientific subroutines libraries, or directly as built-in function in mixed symbolic-numerical platforms, such as the function NDSolve of the *Mathematica* platform [24], which implements automatic relative error control schemes. After truncation to sufficiently large finite order N, the desired final solution is then reconstructed as:

$$T(\mathbf{x},t) = \sum_{i=1}^{N} \frac{1}{N_i} \psi_i(\mathbf{x})\bar{T}_i(t) \; + T_F(\mathbf{x},t,T^*) \tag{9}$$

The truncation order N may be adaptively chosen along the numerical integration march, so as to always work with truncation orders that are just enough to satisfy the user prescribed accuracy requirements, at selected positions $(\mathbf{x})$ and time values (t). It should be recalled that the filter problem, in the case of an implicit filtering strategy for nonlinear problems, has to be solved simultaneously with the transformed system, eqs.(8).

3. EIGENVALUE PROBLEM SOLUTION

The eigenvalue problem that provides the basis for the eigenfunction expansion can be efficiently solved through the generalized integral transform technique itself, as proposed in [13,22] and successfully employed in several applications. The idea is to employ the generalized integral transform technique formalism to reduce the eigenvalue problem described by partial differential equations into standard algebraic eigenvalue problems, which can be solved by existing routines for matrix eigensystem analysis. Therefore, the eigenfuctions of the original auxiliary problem can be expressed by eigenfunction expansions based on a simpler auxiliary eigenvalue problem, for which exact analytic solutions are available.

The solution of problem (5) is thus itself proposed as an eigenfunction expansion:

$$\psi_i(\mathbf{x}) = \sum_{n=1}^{\infty} \tilde{\Omega}_n(\mathbf{x})\bar{\psi}_{i,n}, \qquad \textit{inverse} \tag{10.a}$$

$$\bar{\psi}_{i,n} = \int_V \hat{w}(\mathbf{x})\psi_i(\mathbf{x})\tilde{\Omega}_n(\mathbf{x})dV, \qquad \textit{transform} \tag{10.b}$$

where

$$\tilde{\Omega}_n(\mathbf{x}) = \frac{\Omega_n(\mathbf{x})}{\sqrt{N_{\Omega n}}} \text{ , with } \quad N_{\Omega_n} = \int_V \hat{w}(\mathbf{x})\Omega_n^2(\mathbf{x})dV \tag{10.c,d}$$

in terms of a simpler auxiliary eigenvalue problem, given as:

$$\nabla.\hat{k}(\mathbf{x})\nabla\Omega_n(\mathbf{x})+(\lambda_n^2\hat{w}(\mathbf{x})-\hat{d}(\mathbf{x}))\Omega_n(\mathbf{x})=0,\ \mathbf{x}\in V \tag{11.a}$$

with boundary conditions

$$\alpha(\mathbf{x})\Omega_n(\mathbf{x})+\beta(\mathbf{x})\hat{k}(\mathbf{x})\frac{\partial\Omega_n(\mathbf{x})}{\partial\mathbf{n}}=0,\quad \mathbf{x}\in S \tag{11.b}$$

where the coefficients, $\hat{w}(\mathbf{x}),\hat{k}(\mathbf{x}),$ and $\hat{d}(\mathbf{x}),$ are simpler forms of the equation coefficients chosen so as to allow for an analytical solution of the auxiliary problem. Thus, the solution of problem (5), which needs to be known in terms of the eigenfunctions $\Omega_n(\mathbf{x})$ and related eigenvalues λ_n, offers a basis itself for the eigenfunction expansion of the original eigenvalue problem (5). Equation (5a) is now operated on with $\int_V\tilde{\Omega}_i(\mathbf{x})(\cdot)dV$, to yield the transformed algebraic system:

$$(\mathbf{A}+\mathbf{C})\{\bar{\boldsymbol{\psi}}\}=\mu^2\mathbf{B}\{\bar{\boldsymbol{\psi}}\} \tag{12.a}$$

with the elements of the M x M matrices given by:

$$\begin{aligned}A_{ij}=&\int_S\frac{\tilde{\Omega}_i(\mathbf{x})-\hat{k}(\mathbf{x})\dfrac{\partial\tilde{\Omega}_i(\mathbf{x})}{\partial\mathbf{n}}}{\alpha(\mathbf{x})+\beta(\mathbf{x})}dS-\int_S\left(k(\mathbf{x})-\hat{k}(\mathbf{x})\right)\tilde{\Omega}_i(\mathbf{x})\frac{\partial\tilde{\Omega}_j(\mathbf{x})}{\partial\mathbf{n}}dS+\\&\int_V\left(k(\mathbf{x})-\hat{k}(\mathbf{x})\right)\nabla\tilde{\Omega}_i(\mathbf{x})\cdot\nabla\tilde{\Omega}_j(\mathbf{x})dV+\int_V\left(d(\mathbf{x})-\hat{d}(\mathbf{x})\right)\tilde{\Omega}_i(\mathbf{x})\tilde{\Omega}_j(\mathbf{x})dV\end{aligned} \tag{12.b}$$

$$C_{ij}=\lambda_i^2\delta_{ij}\,;\qquad\qquad B_{ij}=\int_V w(\mathbf{x})\tilde{\Omega}_i(\mathbf{x})\tilde{\Omega}_j(\mathbf{x})dV \tag{12.c,d}$$

where δ_{ij} is the Kronecker delta.

Therefore, the eigenvalue problem given by Eqs. (5) is reduced to the standard algebraic eigenvalue problem given by Eqs. (12), which can be solved with existing software for matrix eigensystem analysis, yielding the eigenvalues μ, whereas the corresponding calculated eigenvectors from this numerical solution, $\bar{\psi}_i$, are to be used in the inversion formula, given by Eq. (10.a), to find the desired eigenfunction, by increasing the number of terms in the truncated expansion, M, to within a prescribed accuracy.

The eigenfunctions $\Omega_n(\mathbf{x})$, may be derived via separation of variables for a general multidimensional formulation, and the separated problems directly obtained from tabulated solutions of classical eigenvalue problems or computed from the ordinary differential equations via modern symbolic platforms. For a cartesian coordinates system, the auxiliary eigenfunctions would be written as:

$$\Omega_n(\mathbf{x})=\mathrm{X}_m(x).\Upsilon_p(y).\mathrm{Z}_q(z) \tag{13}$$

However, for convergence improvement purposes, it is of interest to include as much information as possible of the coefficients spatial behavior into the auxiliary one-dimensional eigenvalue problems. This is particularly important when multiple spatial scales and/or very abrupt variations of the coefficients need to be handled. In such cases, an integral balance procedure [25-26] can be particularly beneficial in accelerating the convergence of the eigenfunctions through improving the spatial resolution of the auxiliary eigenfunctions. Therefore, in order to illustrate the integral balance procedure for an arbitrary one-dimensional auxiliary problem, let us consider the following Sturm-Liouville problem:

$$\frac{d}{dx}\left[k_x(x)\frac{d\mathrm{X}(x)}{dx}\right]+[\gamma^2w_x(x)-d_x(x)]\mathrm{X}(x)=0,\ x_0\le x\le x_1 \tag{14.a}$$

with boundary conditions

$$\begin{aligned}&\alpha_{x,0}\mathrm{X}(x)-\beta_{x,0}k_x(x)\frac{d\mathrm{X}(x)}{dx}=0,\quad x=x_0\\&\alpha_{x,1}\mathrm{X}(x)+\beta_{x,1}k_x(x)\frac{d\mathrm{X}(x)}{dx}=0,\quad x=x_1\end{aligned} \tag{14.b,c}$$

The integral balance procedure employed is a convergence acceleration technique [25-26] that is here aimed at obtaining eigenfunction expansions of improved convergence behavior for both the eigenfunction and its spatial derivative, through integration over the domain of the problem, thus benefiting from the better convergence characteristics of the integrals of eigenfunction expansions. It consists of the double integration of the original equation that governs the potential for which the convergence improvement is being sought, in this case, the eigenvalue problem itself, Eq.(14.a). Through a single integration of the original equation, an improved expression for the eigenfunction derivative is obtained, and a second integration then offers an improved relation for computation of the eigenfunction itself. However, the problem boundary conditions need to be accounted for, so that the eigenfunctions and respective derivatives at the boundaries can be eliminated.

The first step is then the integration of Eq.(14.a) with $\int_{x_0}^{x} (.)\, dx$ to find:

$$\frac{d\mathrm{X}(x)}{dx} = \frac{1}{k_x(x)} k_x(x_0) \left.\frac{d\mathrm{X}(x)}{dx}\right|_{x_0} - \frac{1}{k_x(x)} \gamma^2 Iw_{x_0}(x) + \frac{1}{k_x(x)} Id_{x_0}(x) \tag{15.a}$$

where

$$Iw_{x_0}(x) = \int_{x_0}^{x} w_x(x')\mathrm{X}(x')\, dx'; \quad Id_{x_0}(x) = \int_{x_0}^{x} d_x(x')\mathrm{X}(x')\, dx' \tag{15.b,c}$$

A second integration over Eq.(15.a) is then performed with $\int_{x}^{x_1} (.)\, dx$ to yield:

$$\mathrm{X}(x) = \mathrm{X}(x_1) - k_x(x_0) \left.\frac{d\mathrm{X}(x)}{dx}\right|_{x_0} Ik_{x_1}(x) + \gamma^2 Iwk_{x_1}(x) - Idk_{x_1}(x) \tag{16.a}$$

where

$$Ik_{x_1}(x) = \int_{x}^{x_1} \frac{1}{k_x(x')}\, dx'; Iwk_{x_1}(x) = \int_{x}^{x_1} \frac{1}{k_x(x')}\, Iw_{x_0}(x')dx'; Idk_{x_1}(x) = \int_{x}^{x_1} \frac{1}{k_x(x')}\, Id_{x_0}(x')dx' \tag{16.b-d}$$

A similar procedure could be implemented by starting from the integration of Eq.(14.a) with $\int_{x}^{x_1} (.)\, dx$ to find:

$$\frac{d\mathrm{X}(x)}{dx} = \frac{1}{k_x(x)} k_x(x_1) \left.\frac{d\mathrm{X}(x)}{dx}\right|_{x_1} + \frac{1}{k_x(x)} \gamma^2 Iw_{x_1}(x) - \frac{1}{k_x(x)} Id_{x_1}(x) \tag{17.a}$$

where

$$Iw_{x_1}(x) = \int_{x}^{x_1} w_x(x')\mathrm{X}(x')\, dx'; \quad Id_{x_1}(x) = \int_{x}^{x_1} d_x(x')\mathrm{X}(x')\, dx' \tag{17.b,c}$$

A second integration over Eq.(17.a) is now performed with $\int_{x_0}^{x} (.)\, dx$ to yield:

$$\mathrm{X}(x) = \mathrm{X}(x_0) + k_x(x_1) \left.\frac{d\mathrm{X}(x)}{dx}\right|_{x_1} Ik_{x_0}(x) + \gamma^2 Iwk_{x_0}(x) - Idk_{x_0}(x) \tag{18.a}$$

where

$$Ik_{x_0}(x) = \int_{x_0}^{x} \frac{1}{k_x(x')}\, dx'; Iwk_{x_0}(x) = \int_{x_0}^{x} \frac{1}{k_x(x')}\, Iw_{x_1}(x')dx'; Idk_{x_0}(x) = \int_{x_0}^{x} \frac{1}{k_x(x')}\, Id_{x_1}(x')dx' \tag{18.b-d}$$

Either Eqs.(15.a) or (17.a) can be used as alternative expressions for the eigenfunctions derivatives, while Eqs.(16.a) or (18.a) can be adopted for computing the eigenfunctions, once the boundary conditions are employed to eliminate the values of the eigenfunctions and derivatives at the boundaries. Therefore, writing Eq.(15.a) for $x=x_1$ and Eq.(16.a) for $x=x_0$, the following two equations are obtained:

$$k_x(x_1) \left.\frac{d\mathrm{X}(x)}{dx}\right|_{x_1} = k_x(x_0) \left.\frac{d\mathrm{X}(x)}{dx}\right|_{x_0} - \gamma^2 Iw_{x_0}(x_1) + Id_{x_0}(x_1) \tag{19.a}$$

$$\mathrm{X}(x_0) = \mathrm{X}(x_1) - k_x(x_0) \left.\frac{d\mathrm{X}(x)}{dx}\right|_{x_0} Ik_{x_1}(x_0) + \gamma^2 Iwk_{x_1}(x_0) - Idk_{x_1}(x_0) \tag{19.b}$$

These two relations, together with the boundary conditions, Eqs.(14.b,c), provide four equations for determination of the missing boundary quantities, $X(x_0), X(x_1), X'(x_0), X'(x_1)$, which can be readily solved through symbolic computation in the more general situation of third kind boundary conditions, to yield:

$$\mathrm{X}[\mathrm{x}_0] \to -\frac{\beta_0(\beta_1(\mathrm{Id}_{\mathrm{x}0}[\mathrm{x}_1]-\gamma^2\mathrm{Iw}_{\mathrm{x}0}[\mathrm{x}_1])+\alpha_1(\mathrm{Idk}_{\mathrm{x}1}[\mathrm{x}_0]-\gamma^2\mathrm{Iwk}_{\mathrm{x}1}[\mathrm{x}_0]))}{\alpha_0\beta_1+\alpha_1(\beta_0+\alpha_0\mathrm{Ik}_{\mathrm{x}1}[\mathrm{x}_0])} \tag{20.a}$$

$$\mathrm{X}[\mathrm{x}_1] \to \frac{\beta_1(\alpha_0\mathrm{Idk}_{\mathrm{x}1}[\mathrm{x}_0]-(\beta_0+\alpha_0\mathrm{Ik}_{\mathrm{x}1}[\mathrm{x}_0])(\mathrm{Id}_{\mathrm{x}0}[\mathrm{x}_1]-\gamma^2\mathrm{Iw}_{\mathrm{x}0}[\mathrm{x}_1])-\gamma^2\alpha_0\mathrm{Iwk}_{\mathrm{x}1}[\mathrm{x}_0])}{\alpha_0\beta_1+\alpha_1(\beta_0+\alpha_0\mathrm{Ik}_{\mathrm{x}1}[\mathrm{x}_0])} \tag{20.b}$$

$$\mathrm{X}'[\mathrm{x}_0] \to -\frac{\alpha_0(\beta_1(\mathrm{Id}_{\mathrm{x}0}[\mathrm{x}_1]-\gamma^2\mathrm{Iw}_{\mathrm{x}0}[\mathrm{x}_1])+\alpha_1(\mathrm{Idk}_{\mathrm{x}1}[\mathrm{x}_0]-\gamma^2\mathrm{Iwk}_{\mathrm{x}1}[\mathrm{x}_0]))}{(\alpha_0\beta_1+\alpha_1(\beta_0+\alpha_0\mathrm{Ik}_{\mathrm{x}1}[\mathrm{x}_0]))\mathrm{k}_\mathrm{x}[\mathrm{x}_0]} \tag{20.c}$$

$$\mathrm{X}'[\mathrm{x}_1] \to \frac{\alpha_1(-\alpha_0\mathrm{Idk}_{\mathrm{x}1}[\mathrm{x}_0]+(\beta_0+\alpha_0\mathrm{Ik}_{\mathrm{x}1}[\mathrm{x}_0])(\mathrm{Id}_{\mathrm{x}0}[\mathrm{x}_1]-\gamma^2\mathrm{Iw}_{\mathrm{x}0}[\mathrm{x}_1])+\gamma^2\alpha_0\mathrm{Iwk}_{\mathrm{x}1}[\mathrm{x}_0])}{(\alpha_0\beta_1+\alpha_1(\beta_0+\alpha_0\mathrm{Ik}_{\mathrm{x}1}[\mathrm{x}_0]))\mathrm{k}_\mathrm{x}[\mathrm{x}_1]} \tag{20.d}$$

In the particular cases of either first or second kind boundary conditions, at one or both boundaries, the final expressions become much simpler. Equations (20) can then be directly substituted into Eqs. (15.a, 16.a) or Eqs. (17.a, 18.a) to finally reach the general working expressions for the eigenfunctions and related spatial derivatives, which account for the local space variations of the equation coefficients (w, k, d) and boundary condition coefficients (α, β).

The expressions so obtained for the eigenfunctions and their derivatives, with improved convergence behavior, can now be employed in the solution of eigenvalue problem (14), making use of the integral transformation procedure, yielding the corresponding transformed algebraic eigenvalue which provides the eigenvalues γ^2 and the eigenvectors that can be readily substituted back in the integral balance expressions and inverse formula. This procedure is detailed in the next section for the application that illustrates this work.

4. APPLICATION

An example of variable coefficients with large but continuous scale changes is drawn from the literature related to the heat transfer analysis of functionally graded materials (FGM) [3]. The related dimensionless energy equation and initial and boundary conditions for the example are written as [3]:

$$w(x)\frac{\partial T(x,t)}{\partial t}=\frac{\partial}{\partial x}[k(x)\frac{\partial T(x,t)}{\partial x}],\ 0<x<1,\quad t>0 \tag{21a}$$

with initial and boundary conditions

$$T(x,0)=f(x),\quad 0<x<1 \tag{21b}$$

$$T(0,t)=0,\quad T(1,t)=0,\quad t>0 \tag{21c,d}$$

where the thermophysical properties are assumed to vary exponentially for this FGM example, in the form [3]:

$$k(x)=k_0e^{2\beta x},\quad w(x)=w_0e^{2\beta x},\quad \alpha_0=\frac{k_0}{w_0}=const. \tag{22a-c}$$

This particular choice of functional forms leads to a problem formulation that allows for an exact solution via the classical integral transform method [27], yielding a benchmark solution for the variable coefficients case. This application was solved for extreme values of the parameter β, with the initial condition given by:

$$f(x)=\frac{1-e^{2\beta(1-x)}}{1-e^{2\beta}} \tag{23}$$

which corresponds to the steady-state solution for the case of prescribed temperatures $T(0,t)=1$ and $T(1,t)=0$. The preferred eigenvalue problem for the solution of problem (21) through the GITT is:

$$\frac{d}{dx}\left(k(x)\frac{dX(x)}{dx}\right)+\gamma^2w(x)X(x)=0 \tag{24.a}$$

$$X(0)=0\ ,\quad X(1)=0 \tag{24.b,c}$$

In this case, the expressions for the eigenfunctions and their derivatives, as computed from the integral balance scheme are simplified to:

$$X(x)=Iwk_{x1}(x)\gamma^2-\frac{Ik_{x1}(x)Iwk_{x1}(0)}{Ik_{x1}(0)}\gamma^2 \tag{25.a}$$

$$\frac{dX(x)}{dx}=\frac{\gamma^2}{k(x)}\left[-Iw_{x0}(x)+\frac{Iwk_{x1}(0)}{Ik_{x1}(0)}\right] \tag{25.b}$$

Substituting the corresponding expressions for $Iwk_{x1}(x)$ and $Iw_{x0}(x)$ and employing the inversion formula, Eq. (10.a), for the original eigenfunctions appearing on the rhs of eqs. (25.a,b) one obtains:

$$X_i(x)=\gamma_i^2\sum_n\bar{X}_{in}IB_n(x)-\gamma_i^2\frac{Ik_{x1}(x)}{Ik_{x1}(0)}\sum_n\bar{X}_{in}IB_n(0) \tag{26.a}$$

$$\frac{dX_i(x)}{dx}=-\frac{\gamma_i^2}{k(x)}\sum_n\bar{X}_{in}IA_n(x)+\frac{\gamma_i^2}{k(x)Ik_{x1}(0)}\sum_n\bar{X}_{in}IB_n(0) \tag{26.b}$$

with $IA_n(x)$ and $IB_n(x)$ given by:

$$IA_n(x) = \int_0^x w(x')\tilde{\Omega}_n(x')dx' \tag{26.c}$$

$$IB_n(x) = \int_x^1 \frac{1}{k(x')} IA_n(x') \tag{26.d}$$

where the eigenfunctions $\Omega(x)$ come from a simpler auxiliary eigenvalue problem with known solution. For this application we have:

$$\frac{d\Omega(x)}{dx} + \lambda^2\Omega(x) = 0 \tag{27.a}$$

$$\Omega(0) = 0\,, \quad \Omega(1) = 0 \tag{27.b,c}$$

with

$$\tilde{\Omega}_n(x) = \frac{\Omega_n(x)}{N^{1/2}_{\Omega n}}\,, \quad N_{\Omega n} = \int_0^1 \Omega^2{}_n(x)dX \tag{28.a,b}$$

The integral transformation of the eigenvalue problem (24) can be achieved by operating on Eq. (24.a) with $\int_0^1 (\cdot)\tilde{\Omega}_m(x)dx$ to obtain

$$\int_0^1 \frac{d}{dx}\left(k(x)\frac{dX_i(x)}{dx}\right)\tilde{\Omega}_m(x)dx + \gamma^2\int_0^1 w(x)X_i(x)\tilde{\Omega}_m(x)dx = 0 \tag{29}$$

employing integration by parts on the first term, and making use of the boundary conditions given by Eqs. (24.b,c), it can be written more conveniently as

$$-\int_0^1 k(x)\frac{dX_i(x)}{dx}\frac{d\tilde{\Omega}_m(x)}{dx}dx + \gamma^2\int_0^1 w(x)X_i(x)\tilde{\Omega}_m(x)dx = 0 \tag{30}$$

and now substituting the expressions for the eigenfunctions and their derivatives with improved convergence, given by Eqs. (26.a,b) into Eq. (30), and truncating the expansions to a finite order *M*, yields the following algebraic eigenvalue problem:

$$\left(\mathbf{A} - \gamma^2\mathbf{B}\right)\bar{\mathbf{X}} = 0 \tag{31a}$$

where

$$\mathbf{A} = \mathbf{A}_1 - \mathbf{A}_2\,, \quad \mathbf{B} = \mathbf{B}_2 - \mathbf{B}_1 \tag{31.b,c}$$

with the matrices coefficients given by:

$$A_{1n,m} = \int_0^1 IA_n(x)\frac{d\tilde{\Omega}_m(x)}{dx}dx\,, \quad A_{2n,m} = \frac{IB_n(0)}{Ik_{x1}(0)}\int_0^1 \frac{d\tilde{\Omega}_m(x)}{dx}dx \tag{31.d,e}$$

$$B_{1n,m} = \int_0^1 w(x)IB_n(x)\tilde{\Omega}_m(x)dx\,, \quad B_{2n,m} = \frac{IB_n(0)}{Ik_{x1}(0)} = \int_0^1 Ik_{x1}(x)w(x)\tilde{\Omega}_m(x)dx \tag{31.f,g}$$

The algebraic problem (31) can be numerically solved to provide results for the eigenvalues γ^2 and eigenvectors $\bar{X}_{in}$, upon truncation to a sufficiently large finite order *M*, and then employed into Eqs. (26.a,b) to provide the desired eigenfunctions and their derivatives with improved convergence behavior. Once these eigenfunctions $X_i(x)$ corresponding to eigenvalue problem (24) are made available, problem (21) becomes exactly transformable and the analytical solution for the temperature *T* is straightforward [3].

5. RESULTS AND DISCUSSIONS

The application related to heat conduction across a FGM layer, has been previously solved through the GITT in [3], for a range of the parameter β within [-3, 3]. At the highest value in this interval, β=3, the thermal conductivity at the two boundaries, $k(1)$ and $k(0)$, experiences a ratio of about 400. Here, an even larger value of β=4 is considered, which leads to a ratio $k(1)/k(0)$ of approximately 3000. Therefore, the FGM thermal conductivity would, for instance, vary from a dimensional thermal conductivity of 0.05 W/mºC at x=0, typical of insulating materials, up to a thermal conductivity of 150 W/mºC at x=1, typical of metallic materials.

Besides the exact solution and the GITT solution using the traditional inverse formula for the eigenfunctions and for obtaining the algebraic eigenvalue problem, the integral balance scheme introduced in this work was also employed for obtaining the algebraic eigenvalue problem, yielding eigenvalues and eigenfunctions with improved convergence behavior. In order to illustrate the improvement achieved, we first present in Tables 1.a-c the convergence of the dimensionless temperature at the position x=0.1 and time t=0.01, in the vicinity of the temperature maximum, for increasing values of the truncation order in the temperature expansion, from N=5 to 40, which is sufficient to yield full convergence to all six significant digits here presented. The three tables correspond to increasing values of the eigenvalue problem truncation order, respectively, M=40, 60 and 80. Besides the exact solution and the two alternative GITT solutions, through the usual inversion formulae and via the integral balance scheme, the relative deviations with respect to the exact solution are also presented. It can be observed the improvement in accuracy provided by the increase in the eigenvalue problem truncation order (*M*), which reduces the error on the first 40 eigenvalues and eigenfunctions that are actually employed in the temperature convergence analysis here undertaken. The relative error in the traditional inversion formula drops down from about 0.06% at M=40 to about 0.0075% at M=80, while the integral balance approach drops from 0.0007% to 0% relative error for the same values of *M*. However, more impressive is the improvement allowed for by the integral balance approach in comparison to the plain inverse formula expansion. In general, two additional significant digits of precision are achieved with the use of the approach here proposed, with respect to the inverse formula, which is also fully analytical and readily applicable as here illustrated.

Table 1.a - Comparison of exact solution, GITT via inverse formula, and GITT via integral balance, for the temperature convergence behavior at x=0.1 and t=0.01, with eigenvalue problem truncation order of M=40 .

N	Exact	GITT Inv. Form.	Rel. Error Inv. Form. %	GITT Int. Balance	Rel. Error Int. Balance %
5	0.360318	0.360152	-0.0460438	0.360316	-0.000555%
10	0.456293	0.456017	-0.0604017	0.456288	-0.001096%
15	0.435866	0.435613	-0.0582122	0.435863	-0.000688%
20	0.431986	0.431738	-0.0573906	0.431983	-0.000694%
25	0.432331	0.432078	-0.0585743	0.432326	-0.001157%
30	0.432365	0.432111	-0.0587322	0.432360	-0.001156%
35	0.432363	0.432110	-0.0587213	0.432360	-0.000694%
40	0.432363	0.432110	-0.0587198	0.432360	-0.000694%

Table 1.b - Comparison of exact solution, GITT via inverse formula, and GITT via integral balance, for the temperature convergence behavior at x=0.1 and t=0.01, with eigenvalue problem truncation order of M=60.

N	Exact	GITT Inv. Form.	Rel. Error Inv. Form. %	GITT Int. Balance	Rel. Error Int. Balance %
5	0.360318	0.360269	-0.0136356	0.360318	0.000000%
10	0.456293	0.456211	-0.0178736	0.456292	-0.000219%
15	0.435866	0.435789	-0.0176817	0.435866	0.000000%
20	0.431986	0.43191	-0.0175531	0.431986	0.000000%
25	0.432331	0.432254	-0.0177952	0.432330	-0.000231%
30	0.432365	0.432287	-0.0178232	0.432364	-0.000231%
35	0.432363	0.432286	-0.0178224	0.432363	0.000000%
40	0.432363	0.432286	-0.0178224	0.432363	0.000000%

Table 1.c - Comparison of exact solution, GITT via inverse formula, and GITT via integral balance, for the temperature convergence behavior at x=0.1 and t=0.01, with eigenvalue problem truncation order of M=80.

N	Exact	GITT Inv. Form.	Rel. Error Inv. Form. %	GITT Int. Balance	Rel. Error Int. Balance %
5	0.360318	0.360297	-0.00572231	0.360318	0.000000%
10	0.456293	0.456259	-0.00750005	0.456293	0.000000%
15	0.435866	0.435834	-0.0074885	0.435866	0.000000%
20	0.431986	0.431954	-0.00745007	0.431986	0.000000%
25	0.432331	0.432298	-0.0075399	0.432331	0.000000%
30	0.432365	0.432332	-0.00754984	0.432364	-0.000231%
35	0.432363	0.432331	-0.00754959	0.432363	0.000000%
40	0.432363	0.432331	-0.00754957	0.432363	0.000000%

This improved convergence behavior is even more evident in the calculation of dimensionless heat fluxes, or temperature derivatives, as shown in Table 2, for the same position and time and increasing truncation orders in the derivative expansions with a fixed *M*= 80. As usual, the derivative expressions are in general slower in convergence than the original potentials, but through the integral balance approach we can observe that at least four significant digits of agreement with the exact solution could be achieved at this truncation order. One should notice that the relative error reached for the derivative employing the integral balance scheme is two orders of magnitude lower than that obtained through the traditional approach. Finally, Table 3 provides an evaluation of the convergence behavior of the temperature distribution by the two approaches throughout the spatial domain, from x=0.01 to 0.9, for fixed truncation orders of N=40 and M=60. Clearly, the integral balance procedure provides final results with 4 to 5 significant digits already fully converged and accurate in comparison to the exact solution.

Table 2 - Comparison of exact solution, GITT via inverse formula, and GITT via integral balance, for the temperature derivative convergence behavior at x=0.1 and t=0.01, with eigenvalue problem truncation order of M=80.

N	Exact	GITT Inv. Form.	Rel. Error Inv. Form. %	GITT Int. Balance	Rel. Error Int. Balance %
5	0.680294	0.678029	-0.33303	0.680289	-0.000735%
10	-2.03037	-2.0343	0.193385	-2.030400	0.001478%
15	-2.78191	-2.78643	0.162484	-2.781950	0.001438%
20	-2.58533	-2.59013	0.185591	-2.585390	0.002321%
25	-2.5561	-2.56094	0.189401	-2.556160	0.002347%
30	-2.55829	-2.56313	0.189241	-2.558350	0.002345%
35	-2.55844	-2.56329	0.189227	-2.558500	0.002345%
40	-2.55844	-2.56328	0.189228	-2.558500	0.002345%

Table 3 - Comparison of exact solution, GITT via inverse formula, and GITT via integral balance, for the temperature along coordinate x and t=0.01, for temperature expansion with N=40 and eigenvalue problem truncation order of M=60.

x	Exact	GITT Inv. Form.	GITT Int. Balance
0.01	0.134336	0.133847	0.134327
0.1	0.432363	0.432286	0.432363
0.2	0.201625	0.201607	0.201625
0.3	0.0904128	0.0904049	0.0904127
0.4	0.0404403	0.040436	0.0404402
0.5	0.0179862	0.0179835	0.0179862
0.6	0.00789693	0.00789506	0.0078969
0.7	0.00336353	0.00336225	0.00336351
0.8	0.00132654	0.00132573	0.00132653
0.9	0.000411261	0.000410878	0.000411252

6. CONCLUSIONS

The integral balance approach, as applied to Sturm-Liouville problems, has been derived and employed in generating improved eigenfunction expressions for the integral transform solution of diffusion problems with space variable coefficients. The proposed approach is aimed at improving the accuracy and convergence rates of eigenfunction expansions when multiscale variations of thermophysical properties and/or geometrical dimensions are present in the problem formulation. The derived expressions explicitly incorporate the space variable coefficients in the final eigenfunction relations, thus providing improved results for the local variations of the eigenfunctions. The critical comparison between the results obtained through the traditional approach and the integral balance scheme demonstrates a significant improvement in the convergence behavior of the solution, allowed for by the approach introduced in this work.

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