On the reduction of computational costs in eigenfunction expansions of multidimensional diffusion problems

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Nomenclature

a^* = rectangular region half-length in the x^* direction
b^* = rectangular region half-length in the y^* direction
B = boundary condition operator, equation (2b)
Bi_k = biot numbers ($k = r, z, x$ or y)
c^* = rectangular region half-length in the z^* direction
$d(\mathbf{x})$ = linear dissipation coefficient, equation (2a)
$f(\mathbf{x})$ = initial condition function, equation (1b)
h_k = heat transfer coefficients ($k = r, z, x$ or y)
k^* = thermal conductivity
K, K_1, K_2 = aspect ratios
$K(\mathbf{x})$ = diffusion coefficient, equation (2a)
L^* = cylinder length
L = equation operator, equation (2a)
$\mathbf{n}$ = outward drawn unit normal vector
N = single-series truncation order
NR, NZ = multiple-series truncation orders
$P(\mathbf{x}, t, T)$ = nonlinear equation source term, equation (1a)
r^*, r = radial co-ordinate, dimensional and dimensionless
r_w^* = cylinder radius
S = boundary surface region
t^*, t = time variable (or corresponding spatial variable), dimensional and dimensionless
$T(\mathbf{x}, t)$ = potential distribution
V = problem (1) spatial domain
$w(\mathbf{x})$ = convection (or storage term) coefficient, equation (1a)
$x^*, \mathbf{x}$ = spatial co-ordinate, dimensional and dimensionless
$\mathbf{x}$ = position vector, problem (1)
y^*, y = spatial co-ordinate, dimensional and dimensionless
z^*, z = spatial co-ordinate, dimensional and dimensionless

Greek symbols

α = thermal diffusivity
α_m = eigenvalue, equation (8)
$\alpha(\mathbf{x})$ = boundary condition coefficient, equation (2b)
β_ℓ = eigenvalue, equation (8)
$\beta(\mathbf{x})$ = boundary condition coefficient, equation (2b)
γ_n = eigenvalue, equation (8)
$\phi(\mathbf{x}, t, T)$ = non-linear boundary equation source term, equation (1c)
μ_i = global eigenvalue, equation (8)
$\psi_i(\mathbf{x})$ = normalized eigenfunctions, problem (4)

Introduction

Eigenfunction expansions are the fundamental tool in the analytical or hybrid numerical-analytical solution of various diffusion and convection-diffusion problems in the engineering sciences. Both in the realm of exact integral transformations or separation of variables of linear problems[1-3], or in the more computationally oriented context of the so-called generalized integral transform technique (GITT) [3-5], the solution is a priori assumed in the form of an eigenfunction expansion, extracted from the basis offered by an associated

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eigenvalue problem, which includes as much information as possible from the original partial differential equation operators. In this sense, different classes of problems were handled through integral transforms, including not only the wide spectrum of diffusion and convection-diffusion, but also eigenvalue problems themselves, boundary layer formulations and Navier-Stokes equations[3-5].

In all such applications, the final solution for the related potential is expressed as double or triple infinite summations for two or three-dimensional transient problems, or a double summation for a three-dimensional steady problem. Each of these summations is associated with the eigenfunction expansion in a corresponding spatial co-ordinate, eliminated through integral transformation from the partial differential system, and recovered analytically through such expressions. From a computational point of view, only a truncated version of such nested summations can be actually evaluated. However, the plain truncation of these series, individually, to a certain prescribed finite order, is certainly not an efficient approach and, to an extent, even a risky one. In this way, some still important information to the final result can be disregarded, while other terms are accounted for that have essentially no contribution to convergence in the relative accuracy required. Therefore, for an efficient computation of these expansions, the infinite multiple summations should first be converted to a single sum representation, with the appropriate re-ordering of terms, according to their individual contribution to the final numerical result. Then, one would be able to evaluate a minimum number of eigenvalues and related derived quantities, such as eigenfunctions, norms, transformed initial conditions and source terms, as many as required to reach the user prescribed accuracy target. This aspect is even more evident in the use of the generalized integral transform technique (GITT), when the computational costs can be markedly reduced through this ordering of terms, which then represents a reduction on the number of ordinary differential equations to be solved numerically in the transformed system.

Since the final solution is not, of course, known a priori, the parameter which shall govern this ordering scheme must be chosen with care, and proved to be a good choice. Also, the ordering scheme itself should not be time consuming or cumbersome, so as to become an attractive feature of this type of approach, allowing that multidimensional applications become as simple and computationally cost-effective as single dimensional situations. Such is the case, as the present work intends to demonstrate in what follows.

Formal solution

The present contribution is first motivated by briefly presenting the formal solution for a sufficiently general non-linear diffusion or convection-diffusion problem, handled through the generalized integral transform technique [3-5]. The practical aspects of the ideas advanced here are then demonstrated through examples.

Therefore, we consider the mathematical formulation below, for the potential $T(\mathbf{x}, t)$, defined within region V and boundary surface S:

$$w(\mathbf{x})\frac{\partial T(\mathbf{x},t)}{\partial t} + LT(\mathbf{x},t) = P(\mathbf{x},t,T)\ , \quad \mathbf{x} \in V\ , \quad t > 0 \tag{1a}$$

with initial and boundary conditions respectively

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

$$BT(\mathbf{x},t) = \phi(\mathbf{x},t,T)\ , \quad \mathbf{x} \in S \tag{1c}$$

where the equation and boundary operators are given by

$$L \equiv -\nabla . K(\mathbf{x})\nabla + d(\mathbf{x}) \tag{2a}$$

$$B \equiv \alpha(\mathbf{x}) + \beta(\mathbf{x})K(\mathbf{x})\frac{\partial}{\partial \mathbf{n}} \tag{2b}$$

with $\alpha(\mathbf{x})$ and $\beta(\mathbf{x})$ being prescribed coefficients that recover the different boundary condition types.

The non-linear equation and boundary source terms, respectively $P(\mathbf{x}, t, T)$ $\phi(\mathbf{x}, t, T)$, may include non-linear portions of the equation and the operators L and B in equations (2) can then be interpreted as characteristic linear representations, eventually, of the original problem operators.

Problem (1) is sufficiently general for the present purposes, and has been solved in previous contributions[3-5]. Summarizing the ideas in the integral transform approach (GITT), the formal solution is written as an eigenfunction expansion, in the form:

$$T(\mathbf{x},t) = \sum_{i=1}^{\infty} \psi_i(\mathbf{x})\bar{T}_i(t) \tag{3}$$

where the normalized eigenfunctions, ψ_is , are obtained from the following auxiliary Sturm-Liouville problem

$$L\psi_i(\mathbf{x}) = \mu_i^2 w(\mathbf{x})\psi_i(\mathbf{x})\ , \quad \mathbf{x} \in V \tag{4a}$$

with boundary conditions

$$B\psi_i(\mathbf{x}) = 0\ , \quad \mathbf{x} \in S \tag{4b}$$

while the transformed potentials, $\bar{T}_i$s , are computed from the non-linear initial value problem

$$\frac{d\bar{T}_i}{dt} + \mu_i^2 \bar{T}_i(t) = \bar{g}_i(t, \bar{T}_j)\ , \quad i, j = 1,2,\ldots, \quad t > 0 \tag{5a}$$

with initial conditions

$$\bar{T}_i(0) = \bar{f}_i \tag{5b}$$

where,

$$\bar{g}_i(t,\bar{T}_j) = \int_V \psi_i(x)P(\mathbf{x},t,T)dv + \int_S \phi(\mathbf{x},t,T)\left[\frac{\psi_i(\mathbf{x}) - K(\mathbf{x})\dfrac{\partial\psi_i}{\partial\mathbf{n}}}{\alpha(\mathbf{x}) + \beta(\mathbf{x})}\right]ds \tag{5c}$$

$$\bar{f}_i = \int_V \psi_i(\mathbf{x})f(\mathbf{x})dv \tag{5d}$$

Therefore, the numerical evaluation of the final solution (3), requires prior computation of the eigenvalues, μ_is, normalized eigenfunctions, ψ_is, as well as the related volume and surface integrals appearing in the transformed source term and initial condition expressions, equations (5c,d), including the evaluation of the normalization integral

$$N_i = \int_V w(\mathbf{x})\psi_i^2(\mathbf{x})dv \tag{5e}$$

required in the definition of the normalized eigenfunction, i.e.

$$\psi_i(\mathbf{x}) = \frac{\tilde{\psi}_i(\mathbf{x})}{N_i^{1/2}} \tag{5f}$$

Only then system (5) is assembled and numerically solved through well-established ODE solvers, with automatic relative error control schemes[6].

For computational purposes, the formal representation in equation (3) is actually truncated to a finite order N, which should suffice to satisfy the user prescribed global accuracy target. Thus, in light of the various steps in the calculations, as above discussed, it is of interest to keep N as small as possible, for improved computational efficiency.

In a one-dimensional application, the eigenvalue problem (4) reduces into an ordinary differential equation, which is handled through the integral transform method itself[3-5], and the formal solution is simply written as:

$$T(x,t) = \sum_{i=1}^{\infty} \psi_i(x)\bar{T}_i(t) \tag{6a}$$

which is then truncated to order N for numerical evaluation.

On the other hand, in two-and three-dimensional situations, the eigenvalue problem (4) becomes a partial differential system itself and, either separable or not, it is solved through secondary eigenfunction expansions in each of the spatial co-ordinates that compose the position vector **x**. For these cases,

solution (3) for a problem described in the cartesian co-ordinate system is then given by:

$$T(x,y,t) = \sum_{m=1}^{\infty} \sum_{n=1}^{\infty} X_m(x) Y_n(y) \bar{T}_{m,n}(t) \tag{6b}$$

for a two-dimensional problem, and by

$$T(x,y,z,t) = \sum_{m=1}^{\infty} \sum_{n=1}^{\infty} \sum_{\ell=1}^{\infty} X_m(x) Y_n(y) Z_\ell(z) \bar{T}_{m,n,\ell}(t) \tag{6c}$$

for a three dimensional problem, where X_m, Y_n and Z_ℓ are eigenfunctions in each of the spatial co-ordinates present in the specific problem definition.

There is a natural, but erroneous, tendency of truncating each of the expansions on equations (6b or 6c), to individual finite orders in each direction, i.e. N_x N_y and N_z, when seeking final converged results from these expressions. The total number of terms in these series then becomes the product of the individual truncation orders, for instance, $N = N_x N_y N_z$ for equation (6.c). This number also represents the total number of coupled ODEs in system (5), and can obviously make the ODE system numerical solution untractable, even for reasonably low individual truncation orders, N_x, N_y and N_z. Nevertheless, the convergence of the two- and three-dimensional solutions should be as feasible as the one-dimensional case, sometimes even with improved rates (lower values of the total truncation order, N).

It then becomes clear that the appropriate way of performing these computations in multidimensional applications must involve a re-organization of the multi-series representations of equations (6b,c), into a single series representation, as in the formal solution, equation (3), with an adequate ordering scheme, that accounts, progressively, with the most important terms to the final converged numerical result. The convergence is governed, mainly, by the behaviour of the transformed potentials, $\bar{T}_i(t)$, at each value of t considered. These functions are expected to decrease in modulus as the order i is increased, until very little contribution to the final numerical result remains within the accuracy target requested, providing the adequate truncation order N. Since the transformed potentials can not possibly be known a priori, being part of the numerical solution of the truncated version of system (5), the ordering scheme should be based on well behaved and simple to calculate estimates of these quantities. For a homogeneous problem ($\bar{g}_i \equiv 0$), system (5) is readily solved in explicit form to yield:

$$\bar{T}_{i,h}(t) = \bar{f}_i e^{-\mu_i^2 t} \tag{7}$$

which represents the best convergence rates achievable for this eigenfunction expansion approach. Therefore, it appears reasonable to follow this governing pattern to implement the ordering scheme in the general situation of non-

homogeneous problems. Considering that the exponential decaying behaviour bounds from below the convergence rates of solution (3), it suffices to organize the eigenvalues, μ_is, in ascending order and, as a consequence, all the other related quantities, to reach a simple and effective scheme for transforming the multiple summations of equations (6b,c) into a single summation, such as in equation (3). Therefore, prior to evaluating all the related quantities from problem (4) and solving system (5), the individual eigenvalues from each expansion should be squared and summed, for the appropriate subsequent ordering. For the three-dimensional case, for instance, one has

$$\mu_i^2 = \alpha_m^2 + \gamma_n^2 + \beta_\ell^2 \tag{8}$$

where α_m, γ_n and β_ℓ are the respective eigenvalues in each spatial co-ordinate, x y and z. Thus, to each order i of the single series representation, corresponds a combination of the individual orders in the multiple series expression (6c), i.e. (m, n, ℓ), and ease associative relations need to be stored within the ordering scheme for future use. Also, the number of individual eigenvalues computed during the procedure should be minimized, especially for situations when the eigenvalues are not explicitly provided from simple analytical expressions.

Once the ordering is completed, the remainder of the computational procedure becomes as straightforward and cost-effective as in the one-dimensional case. In fact, except for the additional effort in the evaluation of double and/or triple integrals, when required to be numerically computed, finding a multidimensional solution requires essentially the same order of CPU time as in a plain one-dimensional situation, with the present integral transform approach.

These ideas and the associated algorithms are now more closely discussed through examples.

Applications

We illustrate the proposed scheme by using examples of heat conduction problems in two and three dimensions in rectangular and cylindrical co-ordinates, that allow for an exact solution[1]. Such problems have practical applications for instance, in the quenching of metallic elements, which are considered to be initially at a uniform temperature T_0^* and are suddenly immersed in a coolant bath at a uniform and constant temperature T_∞^*. The elements are supposed homogeneous and isotropic, with no intern heat sources, and physical properties are assumed constant in the range of temperature.

Two-dimensional problem in cylindrical co-ordinates

We consider transient heat conduction in a cylinder of length L^* and radius r_w^*. The formulation of this problem, in dimensionless form, taking into account the symmetry with respect to the cylinder axis and to the plane $z^* = 0$, is given by:

$$\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial\theta(r,z,t)}{\partial r}\right)+\frac{1}{K^2}\frac{\partial^2\theta(r,z,t)}{\partial z^2}=\frac{\partial\theta(r,z,t)}{\partial t},\quad \text{in } 0<r<1,\ 0<z<1 \text{ and } t>0 \tag{9a}$$

subjected to the initial and boundary conditions:

$$\theta(r,z,0)=1,\quad \text{in}\quad 0\le r\le 1\quad \text{and}\quad 0\le z\le 1 \tag{9b}$$

$$\left.\frac{\partial\theta}{\partial r}\right|_{r=0}=0,\quad 0\le z\le 1,\quad t>0 \tag{9c}$$

$$\left.\frac{\partial\theta}{\partial r}\right|_{r=1}+Bi_r\theta(1,z,t)=0,\quad 0\le z\le 1,\quad t>0 \tag{9d}$$

$$\left.\frac{\partial\theta}{\partial z}\right|_{z=0}=0,\quad 0\le r\le 1,\quad t>0 \tag{9e}$$

$$\left.\frac{\partial\theta}{\partial z}\right|_{z=1}+Bi_z\theta(r,1,t)=0,\quad 0\le r\le 1,\quad t>0 \tag{9f}$$

where the following dimensionless variables are defined:

$$\theta(r,z,t)=\frac{T^*(r^*,z^*,t^*)-T^*_\infty}{T^*_0-T^*_\infty}\ :\ t=\frac{\alpha t^*}{r^{*2}_w}\ :\ r=\frac{r^*}{r^*_w}\ :\ z=\frac{z^*}{L^*}$$

$$Bi_r=\frac{h_r r^*_w}{k^*}\ :\ Bi_z=\frac{h_z L^*}{k^*}\ :\ K=\frac{L^*}{r^*_w} \tag{10a-g}$$

The exact solution of problem (1) is obtained by separation of variables or integral transforms as [1,2]:

$$\theta(r,z,t)=\sum_{m=1}^{\infty}\sum_{n=1}^{\infty}\left(\frac{1}{N_m.N_n}\right)\left(\frac{1}{\alpha_m.\gamma_n}\right)\sin(\gamma_n)J_1(\alpha_m)J_0(\alpha_m r)\cos(\gamma_n z)\exp(-\mu^2_{m,n}t) \tag{11a}$$

where α_m and γ_n are the eigenvalues associated with the radial and axial directions respectively, and are obtained as the positive roots of the following transcendental equations:

$$\frac{J_1(\alpha_m)}{J_0(\alpha_m)}=\frac{Bi_r}{\alpha_m} \tag{11b}$$

$$\frac{\sin(\gamma_n)}{\cos(\gamma_n)}=\frac{Bi_z}{\gamma_n} \tag{11c}$$

The global eigenvalues, μ_is, are defined as:

$$\mu_i^2 \equiv \mu_{m,n}^2 = \alpha_m^2 + \frac{\gamma_n^2}{K^2} \tag{11d}$$

and N_m and N_n, the normalization integrals associated with the eigenfunctions of the Sturm-Liouville problems, are respectively given by:

$$N_m = \frac{1}{2} J_0^2(\alpha_m)\left(1+\left(\frac{Bi_r}{\alpha_m}\right)^2\right) = \frac{1}{2} J_1^2(\alpha_m)\left(1+\left(\frac{\alpha_m}{Bi_r}\right)^2\right) \tag{11e}$$

$$N_n = \frac{1}{2}\left(1+\left(\frac{1}{Bi_z}\right)+\left(\frac{\gamma_n}{Bi_z}\right)^2\right)\sin^2(\gamma_n^2) \tag{11f}$$

Two-dimensional problem in rectangular co-ordinates

For this case, we consider the transient heat conduction problem in the rectangular region $-a^* \le x^* \le a, -b^* \le y^* \le b^*$. The formulation of such problem, taking into account the symmetry with respect to the planes $x^* = 0$ and $y^* = 0$, is given in dimensionless form by:

$$\frac{\partial^2\theta(x,y,t)}{\partial x^2} + \frac{1}{K^2}\frac{\partial^2\theta(x,y,t)}{\partial y^2} = \frac{\partial\theta(x,y,t)}{\partial t}, \quad \text{in} \quad 0<x<1, \quad 0<y<1, \quad t>0 \tag{12a}$$

subjected to the initial and boundary conditions:

$$\theta(x,y,0) = 1, \quad \text{in} \quad 0\le x\le 1, \quad 0\le y\le 1 \tag{12b}$$

$$\left.\frac{\partial\theta}{\partial x}\right|_{x=0} = 0, \quad 0<y<1, \quad t>0 \tag{12c}$$

$$\left.\frac{\partial\theta}{\partial x}\right|_{x=1} + Bi_x\theta(1,y,t) = 0, \quad 0<y<1, \quad t>0 \tag{12d}$$

$$\left.\frac{\partial\theta}{\partial y}\right|_{y=0} = 0, \quad 0<x<1, \quad t>0 \tag{12e}$$

$$\left.\frac{\partial\theta}{\partial y}\right|_{y=1} + Bi_y\theta(y,1,t) = 0, \quad 0<x<1, \quad t>0 \tag{12f}$$

where the following dimensionless variables are defined:

$$\theta(x,y,t)=\frac{T^*(x^*,y^*,t^*)-T_\infty^*}{T_0^*-T_\infty^*}\ ;\ x=\frac{x^*}{a^*}\ ;\ y=\frac{y^*}{b^*}\ ;\ t=\frac{\alpha t^*}{a^{*2}}\ ;$$
$$Bi_x=\frac{h_x^* a^*}{k^*}\ ;\ Bi_y=\frac{h_y^* b^*}{k^*}\ ;\ K=\frac{b^*}{a^*} \qquad (13a\text{-}g)$$

The exact solution of problem (12) is obtained as[1,2]:

$$\theta(x,y,t)=\sum_{m=1}^{\infty}\sum_{n=1}^{\infty}\left(\frac{1}{N_m.N_n}\right)\left(\frac{1}{\alpha_m.\gamma_n}\right)\sin(\alpha_m)\sin(\gamma_n)\cos(\alpha_m x)\cos(\gamma_n y)\exp(-\mu_{m,n}^2 t) \qquad (14a)$$

where α_m and γ_n are the eigenvalues associated with the x and y directions respectively, and are obtained as the positive roots of the following transcendental equations:

$$\frac{\sin(\alpha_m)}{\cos(\alpha_m)}=\frac{Bi_x}{\alpha_m} \qquad (14b)$$

$$\frac{\sin(\gamma_n)}{\cos(\gamma_n)}=\frac{Bi_y}{\gamma_n} \qquad (14c)$$

The global eigenvalues, μ_is, are again defined by equation (11d). The normalization integrals N_m and N_n, associated with the eigenfunctions of the Sturn-Liouville problems, are given respectively by:

$$N_m=\frac{1}{2}\left(1+\left(\frac{1}{Bi_x}\right)+\left(\frac{\alpha_m}{Bi_x}\right)^2\right)\sin^2(\alpha_m^2) \qquad (14d)$$

$$N_n=\frac{1}{2}\left(1+\left(\frac{1}{Bi_y}\right)+\left(\frac{\gamma_n}{Bi_y}\right)^2\right)\sin^2(\gamma_n^2) \qquad (14e)$$

Three-dimensional problem in rectangular co-ordinates

The mathematical formulation of the three-dimensional heat conduction problem here considered in the region $-a^* \le x^* \le a^*$, $-b^* \le y^* \le b^*$ and $-c^* \le z^* \le c^*$, is given, in dimensionless form by:

$$\frac{\partial^2\theta(x,y,z,t)}{\partial x^2}+\frac{1}{K_1^2}\frac{\partial^2\theta(x,y,z,t)}{\partial y^2}+\frac{1}{K_2^2}\frac{\partial^2\theta(x,y,z,t)}{\partial z^2}=\frac{\partial\theta(x,y,z,t)}{\partial t}\ ,$$

$$\text{in}\quad 0<x<1,\ 0<y<1,\ 0<z<x<1\quad\text{and}\quad t>0 \qquad (15a)$$

subjected to the initial and boundary conditions:

$$\theta(x,y,z,0) = 1\ , \quad \text{in} \quad 0\le x\le 1\ , \quad 0\le y\le 1\ , \quad 0\le z\le 1 \tag{15b}$$

$$\left.\frac{\partial\theta}{\partial x}\right|_{x=0} = 0, \quad \text{in} \quad 0<y<1, \quad 0<z<1, \quad t>0 \tag{15c}$$

$$\left.\frac{\partial\theta}{\partial x}\right|_{x=1} + Bi_x\theta(1,y,z,t) = 0, \quad \text{in} \quad 0<y<1, \quad 0<z<1, \quad t>0 \tag{15d}$$

$$\left.\frac{\partial\theta}{\partial y}\right|_{y=0} = 0, \quad \text{in} \quad 0<x<1, \quad 0<z<1, \quad t>0 \tag{15e}$$

$$\left.\frac{\partial\theta}{\partial y}\right|_{y=1} + Bi_y\theta(x,1,z,t) = 0, \quad \text{in} \quad 0<x<1, \quad 0<z<1, \quad t>0 \tag{15f}$$

$$\left.\frac{\partial\theta}{\partial z}\right|_{z=0} = 0\ . \quad \text{in} \quad 0<x<1, \quad 0<y<1, \quad t>0 \tag{15g}$$

$$\left.\frac{\partial\theta}{\partial z}\right|_{z=1} + Bi_z\theta(x,y,1,t) = 0\ . \quad \text{in} \quad 0<x<1, \quad 0<y<1, \quad t>0 \tag{15h}$$

where it was taken into account the symmetry with respect to the planes $x^* = 0$, $y^* = 0$ and $z^* = 0$, as evident from boundary conditions (15c), (15e) and (15g), respectively.

In addition to the dimensionless variables defined by equations (13a-g), the following dimensionless quantities are introduced:

$$\theta(x,y,z,t) = \frac{T^*(x^*,y^*,z^*,t^*) - T^*_\infty}{T^*_0 - T^*_\infty}\ ;\ z = \frac{z^*}{c^*}\ ;\ Bi_z = \frac{h^*_z c^*}{k^*}\ ;\ K_1 = \frac{b^*}{a^*}\ ;\ K_2 = \frac{c^*}{a^*} \tag{16a-c}$$

The exact solution of problem (15) is obtained as[1,2]:

$$\theta(x,y,z,t) = \sum_{m=1}^{\infty}\sum_{n=1}^{\infty}\sum_{\ell=1}^{\infty}\left(\frac{1}{N_m.N_n.N_\ell}\right)\left(\frac{1}{\alpha_m.\gamma_n.\beta_\ell}\right)\sin(\alpha_m)\sin(\gamma_n)\sin(\beta_\ell)\cos(\alpha_m x)$$

$$\cos(\gamma_n y)\cos(\beta_\ell z)\exp(-\mu^2_{m,n,\ell}t),$$

$$\text{in} \quad 0\le x\le 1, \quad 0\le y\le 1, \quad 0\le z\le 1, \quad t>0 \tag{17a}$$

where α_m, γ_n and β_ℓ are the eigenvalues associated with the x, y and z directions respectively. The eigenvalues α_m and γ_n are obtained from the solution of equations (14b,c) respectively, while the β_ℓs are the positive roots of

$$\frac{\sin(\beta_\ell)}{\cos(\beta_\ell)} = \frac{Bi_z}{\beta_\ell} \tag{17b}$$

The global eigenvalues μ_is, are defined as:

$$\mu_i^2 \equiv \mu_{m,n,\ell}^2 = \alpha_m^2 + \frac{\gamma_n^2}{K_1^2} + \frac{\beta_\ell^2}{K_2^2} \tag{17c}$$

The normalization integrals N_m and N_n are given by equations (14d,e), respectively, while N_ℓ is given, by analogy, as:

$$N_\ell = \frac{1}{2}\left(1 + \left(\frac{1}{Bi_z}\right) + \left(\frac{\beta_\ell}{Bi_z}\right)^2\right)\sin^2(\beta_\ell^2) \tag{17d}$$

Computational procedure

For computational purposes, the series solutions given by equations (11a), (14a) and (17a) are, in general, truncated to a finite number of terms for each summation, in order to compute the potential θ. The solution convergence is verified by comparing the values for the potential obtained with the truncated series for different numbers of retained terms. Such number of terms is commonly user-supplied and even taken as the same for each summation. This procedure certainly results in unnecessary computational effort owing to the fact that each summation might be converged with a markedly different truncation order. Each term of the series solutions, equations (11a), (14a) and (17a), involves a product of a constant, a periodic function and an exponential in time, where the latter is responsible for the series convergence. Therefore, the most significative terms for the solution convergence are those corresponding to smaller values of μ_i.

The eigenvalues α_m, γ_n and β_ℓ, associated with the auxiliary Sturm-Liouville problems in each of the space variables, are required in equations (11d) and (17c) for the computation of μ_i. Such eigenvalues form an infinite increasing sequence, i.e.

$$\lambda_1 < \lambda_2 < \ldots < \lambda_n < \ldots \qquad (\text{with } \lambda_n \to \infty, \text{when } n \to \infty) \tag{18}$$

where $\lambda = \alpha, \gamma$ or β.

Therefore, in a two-dimensional problem, for instance, we can say that:

$$\mu_{m+i,n} > \mu_{m,n} \tag{19a}$$

$$\mu_{m,n+1} > \mu_{m,n} \tag{19b}$$

and consequently the series terms based on $\mu_{m+1,n}$ and $\mu_{m,n+1}$ are expected to be less significant for the potential convergence as that term based on $\mu_{m,n}$.

We present below an improved scheme where only the most important global eigenvalues are taken into account, in order to reach the converged solution more efficiently. Such scheme minimizes the computation, avoiding terms that do not contribute in increasing the accuracy of the final solution towards the user prescribed precision target.

In the proposed scheme, the multiple nested summations in the series solutions are transformed into a single summation, in order to keep in the truncated series only those terms contributed from the most important global eigenvalues. Such approach is illustrated with the two-dimensional test-case in cylindrical co-ordinates, as described next.

The global eigenvalue $\mu_{m,n}$, computed from equation (11d), can be transformed into a single indexed quantity μ_i, so that there is a one-to-one correspondence between the pair (m, n) and the index i. Therefore, the double summation in equation (11a) is transfomed into the following single summation with index i.

$$\theta(r,z,t) = \sum_{i=1}^{\infty} \left(\frac{1}{N_m \cdot N_n}\right)\left(\frac{1}{\alpha_m \cdot \gamma_n}\right) \sin(\gamma_n) J_1(\alpha_m) J_0(\alpha_m r) \cos(\gamma_n z) \exp(-\mu_i^2 t) \quad (20)$$

The summation in equation (20) is truncated in a finite number of terms. We can assume, initially, that there would be a total of N terms required for convergence in the double summation of equation (3a), or in its equivalent single-series form (20), and take $1 \le m \le NR$ and $1 \le n \le NZ$ where NR = NZ is the integer greater than or equal to $\sqrt{N}$, to start with the ordering procedure.

The proposed scheme consists in searching for ordered pairs (m, n) keeping the evaluation of additional eigenvalues to a minimum. The basic steps of the algorithm are described next:

(1) Set the number of terms (N) required for convergence in the series of equation (20). If there is no previous experience to set an appropriate number initially, set N = 4, so that NR = NZ = 2.

(2) Compute $\mu_{NR,NZ}$.

(3) Search for m′, where m′ is the largest integer satisfying $\mu_{m',1} < \mu_{NR,NZ}$.

(4) Search for n′, where n′ is the largest integer satisfying $\mu_{1,n'} < \mu_{NR,NZ}$.

(5) Compute $\mu_i = \mu_{m,n}$ for $1 \le m \le m'$ and $1 \le n \le n'$ satisfying the requirement $\mu_{m,n} < \mu_{NR,NZ}$.

(6) Compute the potential θ(r, z, t) with equation (20) by using the global eigenvalues μ_i assembled in step 5.

(7) Check for convergence of the potential. If not converged make NR = NR + 1 and NZ = NZ + 1 and return to step 2. In returning to step 3, it should be noticed that several quantities are available from the previous iteration and do not need to be computed again. It should be noted that the convergence test criterion is based on the accumulated contribution of the last three computed terms of the series (in absolute value), in order to avoid false convergence information owing to possible local minima on the eigenfunctions.

The detailed algorithms for two and three-dimensional problems may be provided by the authors on request. The application of the present approach is now illustrated.

Results and discussion

The numerical results obtained with the proposed scheme are presented below, as applied to the solution of the three test-cases previously described.

Two-dimensional problem in cylindrical co-ordinates

This test-case was solved according to the following input data:

- N = 4 (initial guess)
- Aspect ratio: K = 5.0
- Biot numbers: $\begin{cases} Bi_r = 0.1 \\ Bi_z = 0.2 \end{cases}$
- Dimensionless position: $\begin{cases} r = 0.1 \\ z = 0.1 \end{cases}$
- Dimensionless time: t = 0.5
- Accuracy required (relative error) = 10^{-9}

The numerical results obtained progressively from the automatic computational procedure are reproduced below, so as to illustrate the scheme behaviour:

(1) Number of α_ms and γ_ns initially calculated: 2

m, n	α_m	γ_n
1	0.4416817834	0.4328407258
2	3.8577097846	3.2039350012

$\mu_{2,2}^2 = 15.2925327618$

(2) Additional eigenvalues calculated:

m, n	α_m	γ_n
3	7.0298247932	6.3148461226
4	–	9.4459478951
5	–	12.5822646663
6	–	15.7206848748
7	–	18.8601598862
8	–	22.0002391364

Therefore, $m' = 2$ and $n' = 7$

(3) Calculation of all the possible μ_is given by equation (11d), limited by the upper bound $\mu_{2,2}^2$:

i	μ_i^2	m	n
1	0.2025768416	1	1
2	0.6056907775	1	2
3	1.7901740599	1	3
4	3.7641200633	1	4

5	6.5276181631	1	5
6	10.0806798636	1	6
7	14.4233080351	1	7
8	14.8894188259	2	1
9	15.2925327618	2	2

(4) The resulting potential is evaluated ($\theta = \sum_{i=1}^{N} S_i$) to yield:

i	S_i	$\theta(r, z, t)$
1	0.9533083118	0.9533083118
2	–0.0273922143	0.9259160975
3	0.0033690224	0.9292851199
4	–0.0004087103	0.9288764096
5	0.0000303858	0.9289067954
6	0.0000000136	0.9289068090
7	0.0000002633	0.9289065457
8	–0.0000193446	0.9288872012
9	0.0000005558	0.9288877570

(5) Since the convergence criterion was not reached, it is necessary to proceed with a new value for NR and NZ:

NR = NR + 1

NZ = NZ + 1

(6) The new upper bound for the global eigenvalues is, then, $\mu^2_{3,3}$. Since the eigenvalues α_3 and γ_3 are already available, $\mu^2_{3,3}$ is immediately determined as:

$\mu^2_{3,3} = 51.0135278848$

(7) Additional eigenvalues calculated:

m, n	α_m	γ_n
4	10.1832916222	([a])
5	–	([a])
6	–	([a])
7	–	([a])
8	–	([a])
9	–	25.1406962876
10	–	28.2814055464
11	–	31.4222913560
12	–	34.5622056098
13	–	37.7044162114

([a]) Values already calculated in previous steps

(8) Calculation of all possible μ_is, limited by the upper bound $\mu^2_{3,3}$:

i	μ_i^2	m	n
1	0.2025768416	1	1
2	0.6056907775	1	2
3	1.7901740599	1	3
4	3.7641200633	1	4
5	6.5276181631	1	5
6	10.0806798636	1	6
7	14.4233080351	1	7
8	14.8894188259	1	1
9	15.2925327618	2	2
10	16.4770160442	2	3
11	18.4509620476	2	4
12	19.5555036801	1	8
13	21.2144601475	2	5
14	24.7675218480	2	6
15	25.4772671908	1	9
16	29.1101500194	2	7
17	32.1885987850	1	10
18	34.2423456644	2	8
19	39.6894985602	1	11
20	40.1641091751	2	9
21	46.8754407693	2	10
22	47.9799665849	1	12
23	49.4259306665	3	1
24	49.8290446024	3	2
25	51.0135278848	3	3

(9) The resulting potential is evaluated as shown in Table I, and convergence is then achieved to nine digits with N = 16.

It should be noted that the convergence test criterion correctly avoided stopping the series evaluation at N = 13, when false convergence in the ninth digit appears; the criterion based on the accumulation of absolute values of the last three terms of the series, then postpones the indication of convergence to the order N = 16.

Two dimensional problem in rectangular co-ordinates

In this case, the following input data were employed:

- N = 20 (initial guess)
- Aspect ratio: K = 5.0

i	S_i	θ(r, z, t)
1	0.9533083118	0.9533083118
2	–0.0273922143	0.9259160975
3	0.0033690224	0.9292851199
4	–0.0004087103	0.9288764096
5	0.0000303858	0.9289067954
6	0.0000000136	0.9289068090
7	–0.0000002633	0.9289065457
8	–0.0000193446	0.9288872012
9	0.0000005558	0.9288877570
10	–0.0000000684	0.9288876886
11	0.0000000083	0.9288878969
12	0.0000000282	0.9288877252
13	0.0000000006	0.9288877245
14	–0.0000000000	0.9288877245
15	–0.0000000015	0.9288877230
16	–0.0000000000	0.9288877230
17	–0.0000000000	0.9288877231
18	–0.0000000000	0.9288877231

Table I.
Final convergence behaviour of the single-series solution (two-dimensional problem; cylindrical co-ordinates)

- Biot numbers: $\begin{cases} Bi_x = 0.1 \\ Bi_y = 0.2 \end{cases}$
- Dimensionless postition: $\begin{cases} x = 0.1 \\ y = 0.1 \end{cases}$
- Dimensionless time: $t = 0.5$
- Accuracy required: 10^{-9}

The numerical results, as extracted from the ordering scheme, are presented below:

(1) Number of α_ms and γ_ns initially calculated: 4

m, n	α_m	γ_n
1	0.3110528483	0.4328407258
2	3.1730971737	3.2039350012
3	6.2990593581	6.3148461226
4	9.4253759772	9.4459478951

$\mu^2_{4,4} = 92.5953570960$

(2) Additional eigenvalues calculated:

m, n	α_m	γ_n
5	12.5743231628	12.5822646663
6	–	15.7206846748
7	–	18.8601598862

8	–	22.0002391364
9	–	25.1406962876
10	–	28.2814055464
11	–	31.4222913560
12	–	34.5633056098
13	–	37.7044162114
14	–	40.8456009478
15	–	43.9868439318
16	–	47.1281335302
17	–	50.2694609948

(3) Calculation of all the possible μ_is limited by the upper bound $\mu^2_{4,4}$:

i	μ_i^2	m	n
1	0.1042479182	1	1
2	0.5073618541	1	2
3	1.6918451365	1	3
4	3.6657911399	1	4
5	6.4292892398	1	5
6	9.9823509403	1	6
7	10.0760397178	2	1
8	10.4791536537	2	2
9	11.6636369361	2	2
10	13.6375829395	2	4
11	14.3249791117	1	7
12	16.4010810393	2	5
13	19.4571747568	1	8
14	19.9541427398	2	6
15	24.2967709113	2	7
16	25.3789382674	1	9
17	29.4289665563	2	8
18	32.0902698616	1	10
19	35.3507300670	2	9
20	39.5911696369	1	11

(4) The resulting potential is converged to nine digits at N = 17, as shown in Table II.

Three-dimensional problem in rectangular co-ordinates

The input data for this case is given by:

- N = 40
- Aspect ratios: $\begin{cases} K_1 = 1.5 \\ K_2 = 2.5 \end{cases}$

i	S_i	θ(x, y, t)
1	0.9930595963	0.9930595963
2	–0.0285344216	0.9645251747
3	0.0035095047	0.9680346794
4	–0.0004257520	0.9676089266
5	0.0000316529	0.9676405795
6	0.0000000142	0.9676405937
7	–0.0001248026	0.9676457911
8	0.0000035861	0.9675157911
9	–0.0000004411	0.9675193771
10	0.0000000535	0.9675189361
11	–0.0000002743	0.9675189896
12	–0.0000000040	0.9675187153
13	0.0000000294	0.9675187113
14	0.0000000000	0.9675187407
15	0.0000000000	0.9675187407
16	–0.0000000016	0.9675187406
17	0.0000000000	0.9675187392
18	0.0000000000	0.9675187392
19	0.0000000000	0.9675187392

Table II.
Final convergence behaviour of the single-series solution (two-dimensional problem; rectangular co-ordinates)

- Biot numbers: $\begin{cases} Bi_x = 0.1 \\ Bi_y = 0.2 \\ Bi_y = 0.3 \end{cases}$
- Dimensionless position: $\begin{cases} x = 0.1 \\ y = 0.1 \\ z = 0.1 \end{cases}$
- Dimensionless time: $t = 0.5$
- Accuracy required (relative error) = 10^{-9}

(1) Number of α_ms, γ_ns and β_ℓs initially calculated: 3

i	α_m	γ_m	β_ℓ
1	0.3110528483	0.4328407199	0.5217911774
2	3.1730971796	3.2039350012	3.2340897570
3	6.2990593581	6.3148461226	6.3305392076

$\mu^2_{3,3,3} = 63.8135013077$

(2) Additional eigenvalues calculated:

i	α_m	γ_m	β_ℓ
4	9.4353759772	9.4459478951	9.4564915612
5	–	12.5822646663	12.5901941738
6	–	–	15.7270363843

7	–	–	18.8654566619
8	–	–	22.0047811342

(3) Calculation of all the possible μ_is, limited by the upper bound $\mu^2_{3,3,3}$. A total of 132 μ_is were found, less than $\mu^2_{3,3,3}$; this number is much larger than in fact necessary, so only the first 40 are presented below, as initially guessed.

i	μ_i^2	m	n	ℓ
1	0.2235835903	1	1	1
2	1.8535148741	1	1	2
3	4.7026273249	1	2	1
4	6.3325586087	1	2	2
5	6.5921372905	1	1	3
6	10.1953754270	2	1	1
7	11.0711818251	1	2	3
8	11.8253067108	2	1	2
9	14.4880582485	1	1	4
10	14.6744191616	2	2	1
11	16.3043504454	2	2	2
12	16.5639291272	2	1	3
13	17.8635526850	1	3	1
14	18.9671019831	1	2	4
15	19.4934839687	1	3	2
16	21.0429728618	2	2	3
17	24.2321063852	1	3	3
18	24.4598500852	2	1	4
19	25.5420993186	1	1	5
20	27.8353445216	2	3	1
21	28.9388938198	2	2	4
22	29.4652758054	2	3	2
23	30.0211430533	1	2	5
24	32.1280273432	1	3	4
25	34.2038982219	2	3	3
26	35.5138911553	2	1	5
27	39.7543687741	1	1	6
28	39.7962860562	1	4	1
29	39.8049785129	3	1	1
30	39.9929348899	2	2	5
31	41.4262173400	1	4	2
32	41.4349097967	3	1	2
33	42.0998191798	2	3	4
34	43.1820684133	1	3	5
35	44.2334125087	1	2	6

36	44.2840222475	3	2	1
37	45.9139535313	3	2	2
38	46.1648397564	1	4	3
39	46.1735322131	3	1	3
40	49.7261606108	2	1	6

(4) The resulting potential is then computed, and found to be converged to nine digits for N = 18 (Table III).

It is noticeable in all the three sets of results, tables I to III, that the present choice of ordering strategy, based on the argument of the dominating exponential term, although not always in a monotonic fashion, offers a good compromise between the overall convergence enhancement and simplicity in use.

As a closing remark, it can be recalled that the present algorithm keeps the evaluation of additional eigenvalues to a minimum, avoiding unnecessary increase on computational cost, while reordering the multiple summations into the single-series representation. The computational savings are even more markedly significant in the case of application of the generalized integral transform technique, when the reordering scheme represents savings on the number of ordinary differential equations to be solved simultaneously. In fact, this observation allowed for the conclusion that the overall computational costs in solving multidimensional situations could be of the same order of magnitude

i	S_i	$\theta(x, y, t)$
1	0.973516718	0.9763516718
2	–0.0218080045	0.9545436673
3	–0.0036553007	0.9508883666
4	0.0000816456	0.9509700122
5	0.0004636124	0.9514336246
6	–0.0001227028	0.9513109128
7	–0.0000017357	0.9513091861
8	0.0000027407	0.9513119269
9	–0.0000029235	0.9513090033
10	0.0000004594	0.9513094627
11	–0.0000000103	0.9513094525
12	0.0000000583	0.9513093942
13	0.0000011276	0.9513105218
14	0.0000000109	0.9513105327
15	–0.0000000252	0.9513105078
16	0.0000000002	0.9513105083
17	0.0000000005	0.9513105087
18	0.0000000004	0.9513105121
19	0.0000000034	0.9513105120
20	0.0000000001	0.9513105120
21	0.0000000000	0.9513105120
22	0.0000000000	0.9513105120

Table III.
Final convergence behaviour of the single-series solution (three-dimensional problem; rectangular co-ordinates)

as for a plain one-dimensional version of the same problem. This aspect became one of the most attractive features of the integral transform approach in the solution of multidimensional convection-diffusion problems, together with the automatic global error control capability.

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