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The best approximation method applied to three-dimensional steady-state heat transport

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The best approximation method is extended to the numerical solution of three-dimensional steady-state heat transport problems. Two families of trial functions are used in the numerical solution; namely, harmonic polynomials and constant sources. Numerical approximation error is evaluated by means of approximate boundaries whereby error is visualized as a geometric displacement of the problem boundary. The problem considered is the determination of temperatures within a nuclear reactor.

Key words: Numerical approximation, partial differential equations, generalized Fourier series, approximate boundaries.

INTRODUCTION

The best approximation method

The theoretical development for the subject mathematical model is provided in detail in Hromadka *et al.*;[1] only a brief presentation is provided herein. Let Ω be a region in $\mathcal{R}^m$ with boundary Γ and let $\mathrm{cl}(\Omega)$ denote the closure of Ω. Consider the Hilbert space $L_2(\mathrm{cl}(\Omega), \mathrm{d}\mu)$, which has inner-product

$$(f,g) = \int fg \, \mathrm{d}\mu \tag{1}$$

To construct an inner-product for the development of a generalized Fourier series, the measure μ is chosen where μ is the measure μ_1 on Ω and another measure μ_2 on Γ. One choice for a plane region is to let μ_1 be the usual two-dimensional Lebesque measure $\mathrm{d}\Omega$ on Ω and μ_2 be the usual arc length measure $\mathrm{d}\Gamma$ on Γ. Then

$$(f,g) = \int_\Omega fg \, \mathrm{d}\Omega + \int_\Gamma fg \, \mathrm{d}\Gamma \tag{2}$$

defines an inner-product.[2]

Consider a boundary value problem consisting of an operator L defined on domain $D(L) \subset L_2(\Omega)$ and mapping onto $L_2(\Omega)$, and a boundary condition operator B defined on a domain $D(B) \subset L_2(\Gamma)$ and mapping onto $L_2(\Gamma)$. The domains of L and B are such that for f in $D(L)$, Lf is in $L_2(\Omega)$, and for f in $D(B)$, Bf is in $L_2(\Gamma)$. (For example, we could have $Lf = \nabla^2 f$, and $Bf(s)$ equals the, almost everywhere (a.e.), radial limit of f at the point s on Γ with appropriate domains).

An operator T is constructed which maps its domain $D(T) = D(L) \cap D(B)$ into $L_2(\mathrm{cl}(\Omega))$ by,[4]

$$\begin{aligned} Tf(x) &= Lf(x) \text{ for } x \text{ in } \Omega \\ Tf(s) &= Bf(s) \text{ for } s \text{ on } \Gamma \end{aligned} \tag{3}$$

This operator T on the Hilbert space $L_2(\mathrm{cl}(\Omega))$ incorporates both the operator L and the boundary conditions operator B, and is linear providing that both L and B are linear.

Consider the inhomogeneous equation $Lf = g_1$, with the inhomogeneous boundary conditions $Bf = g_2$, and define a function g on $\mathrm{cl}(\Omega)$ by: $g = g_1$ on Ω; $g = g_2$ on Γ. Then if the solution exists for the operator equation $Tf = g$, the solution f satisfies $\nabla^2 f = g_1$ on Ω and $f = g_2$ on Γ. One approach to the approximate solution of

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$Tf = g$ is to look at a subspace D_n of dimension n, which is contained in $D(T)$, and minimize $\|Th - g\|$ over all h in D_n, such as developed in detail by Hromadka *et al.*[3]

Definition of inner-product and norm

Consider a linear operator relationship $L(\phi) = h$ defined on the problem domain with auxiliary conditions $\phi = \phi_b$ on the boundary Γ. The domain Ω may represent both time and space and ϕ_b may be both initial and boundary conditions.

Choose a set of m linearly independent functions $\{f_i\}_{i=1}^m$. Let S^m be the m-dimensional space spanned by the m elements of $\{f_i\}$.

Define the inner-product (u, v) for $u, v \in S^m$ by

$$(u, v) = \int_\Gamma uv \, d\Gamma + \int_\Omega Lu \, Lv \, d\Omega \tag{4}$$

The associated norm '$\| \|$' is given by

$$\|u\| \equiv (u, u)^{1/2} \tag{5}$$

Using the above inner-product and norm, a generalized Fourier series can be used to find the 'best' approximation $\hat{\phi}_m \in S^m$ of ϕ by constructing a new set of functions $\{g_i\}$, by the orthonormalization of the $\{f_i\}$.

Orthonormalization process

Orthonormal functions $\{g_i\}$ are generated by the well-known Gram-Schmidt procedure using the previous inner-product and norm. That is,

$$\begin{aligned} g_1 &= f_1 / \|f_1\|; \\ &\vdots \\ g_m &= [f_m - (f_m, g_1)g_1 - \cdots - (f_m, g_{m-1})g_{m-1}] \\ &\quad / \|f_m - (f_m, g_1)g_1 - \cdots - (f_m, g_{m-1})g_{m-1}\| \end{aligned} \tag{6}$$

The elements $\{g_i\}$ form a basis for S^m as do the elements of $\{f_i\}$. However, because they are orthogonal, the elements of $\{g_i\}$ can be directly used in the development of a generalized Fourier series where the computed coefficients do not change as the dimension m increases.

Each element $\hat{\phi}_m \in S^m$ is written as:

$$\hat{\phi}_m = \sum_{i=1}^m \gamma_i g_i \tag{7}$$

where $\hat{\phi}_m \in S^m$, and the γ_i are unique real constants.

Generalized Fourier series

The objective is to determine the element $\hat{\phi}_m \in S^m$ such that $\|\hat{\phi}_m - \phi\|^2$ is a minimum, where

$$\begin{aligned} \|\hat{\phi}_m - \phi\|^2 &= \int_\Gamma \left[\sum_{i=1}^m \gamma_i g_i - \phi_b\right]^2 d\Gamma \\ &\quad + \int_\Omega \left[L\sum_{i=1}^m \gamma_i g_i - L\phi\right]^2 d\Omega \\ &= \int_\Gamma \left[\sum_{i=1}^m \gamma_i g_i - \phi_b\right]^2 d\Gamma \\ &\quad + \int_\Omega \left[\sum_{i=1}^m \gamma_i Lg_i - f\right]^2 d\Omega \end{aligned} \tag{8}$$

Therefore, minimizing $\|\hat{\phi}_m - \phi\|^2$ is equivalent to minimizing the sum of the L^2 error in approximating the auxiliary conditions and the L^2 error in approximating the operator relationship. Because the inner-product is well-defined and the $\{g_i\}$ are orthonormalized, the minimizing coefficients γ_i of eqn (7) are the generalized Fourier constants, γ_i^*:

$$\gamma_i^* = (g_i, \phi), \quad i = 1, 2, \ldots, m \tag{9}$$

Thus,

$$\phi_m^* = \sum_{i=1}^m \gamma_i^* g_i = \sum_{i=1}^m (g_i, \phi) g_i \tag{10}$$

is the 'best' approximation of ϕ in the space S^m, from the above definition for the inner-product.

The weighted inner product

In the inner-product of eqn (4), consideration is given to the two basic requirements imposed on the best approximation function $\hat{\phi}_m$ from the space S^m spanned by the m trial functions in $\{f_i\}$. That is, the L^2 error in satisfying the linear operator relationship over Ω is weighted equally as the L^2 error in satisfying the problem's auxiliary conditions.

It can be useful to weight the inner-product terms in order not to bias the approximation in either of the error minimization efforts. For $0 < \epsilon < 1$, one weighting of eqn (4) is:

$$(u, v) = \epsilon \int_\Gamma uv \, d\Gamma + (1 - \epsilon) \int_\Omega Lu \, Lv \, d\Omega \tag{11}$$

In eqn (11), an ϵ-value close to one would force the approximation function $\hat{\phi}_m$ to focus upon satisfying the problem's boundary conditions rather than satisfying the linear operator. Conversely, an ϵ-value close to zero would emphasize the linear operator relationship rather than the boundary conditions.

The general problem

In this paper, a variant of the best approximation method is applied to find an approximate solution $\hat{\phi}_m \in S^m$ to the three-dimensional linear operator equation with boundary conditions:

$$\begin{aligned} L\phi &= 0 \text{ on domain } \Omega \\ \phi &= \phi_b \text{ on boundary } \Gamma \end{aligned} \tag{12}$$

where S^m is the m-dimensional space spanned by the m trial functions $\{f_i\}$.

By a judicious choice of trial functions $\{f_i\}$, the inner-product in eqn (4) can be simplified. In particular, by choosing trial functions $\{f_i\}$ which satisfy the linear operator equation

$$Lf_i = 0 \text{ on } \Omega \text{ for } i = 1, \ldots, m \tag{13}$$

the inner-product in eqn (4) reduces to

$$(f_i, f_j) = \int_\Gamma f_i f_j \, d\Gamma \tag{14}$$

Since only the problem's boundary is used in eqn (14), the inner-product weighting, ϵ, is unnecessary.

Approximation error evaluation — approximate boundary method

If $\hat{\phi}_m$ satisfies the auxiliary conditions in eqn (12) exactly, and the trial functions are chosen that satisfy eqn (13), then $\hat{\phi}_m = \phi$ everywhere on $\Omega \cup \Gamma$. If $\hat{\phi}_m$ is not exact, the least-squares (L^2) error occurs on Γ. This suggests a method of evaluating the error of the approximation. This method, called the approximate boundary method, requires that a new boundary, $\hat{\Gamma}$, be constructed which has the property that (for $\hat{\Omega}$ being the domain enclosed by $\hat{\Gamma}$),

$$\begin{aligned} L\hat{\phi}_m &= 0 \text{ on } \hat{\Omega} \\ \hat{\phi}_m &= \phi_b \text{ on } \hat{\Gamma} \end{aligned} \tag{15}$$

In this way $\hat{\phi}_m$ forms an exact solution to the problem, but with a geometrically transformed domain and boundary. An evaluation of the modeling error can be made by comparing Γ with $\hat{\Gamma}$. Hromadka *et al.*[3] use the approximate boundary to evaluate modeling error for several case studies.

COMPUTER IMPLEMENTATION

A FORTRAN computer program was prepared for three-dimensional analysis of steady-state heat transport. In order to develop the approximation, $\hat{\phi}_m$, each trial function, f_i, is itself approximated as a finite-dimensional vector whose elements are the value of the trial function evaluated at each of a set of evaluation points defined along the problem boundary. In this paper, three-dimensional steady state heat transport is considered, and the trial functions were selected that satisfy the Laplacian equation $\nabla^2(f_i) = 0$ over the problem domain, Ω, thereby making L^2 error minimization necessary only on the boundary, Γ. Because the trial functions f_i are represented by discrete vectors, $\mathbf{F_i}$, all Gram-Schmidt operations between functions are computed by equivalent operations between vectors in $\mathbf{R}^n$. That is, the inner-product of eqn (14) is replaced by the familiar vector dot product of two vectors:

$$(\mathbf{F_i}, \mathbf{F_j}) = \sum_{k=1}^{n} F_{ik} F_{jk} \tag{16}$$

where F_{ik} is the kth component of the ith vector.

The problem boundary is represented as a mesh of n evaluation points stored in a single vector, $\mathbf{G}$. The vectors $\mathbf{F_i}$ are developed by evaluating trial function f_i at each (x, y, z) nodal point stored in vector $\mathbf{G}$.

Upon development of m vectors $\mathbf{F_i}$ (for m trial functions f_i), the computer program then: i) orthonormalizes the trial functions (basis vectors), and ii) computes the coefficients of the 'best approximation', ϕ_m^*. The vectors, $\mathbf{F_i}$, representing the trial functions, are orthonormalized by the familiar Gram-Schmidt process. The resulting orthonormalized vectors are denoted by vectors $\mathbf{G_i}$. Note that the inner-product used is the vector dot product of eqn (16).

Once the m orthonormalized vectors $\mathbf{G_i}$ have been constructed, the generalized Fourier coefficients are computed. The Fourier coefficients are used in back-substitution through the Gram-Schmidt process to find the coefficients of the approximation ϕ_m^*. These final coefficients are written to a file for post-processing in routines that generate the approximate boundaries.

APPLICATION: THREE-DIMENSIONAL STEADY-STATE HEAT TRANSFER

For demonstration purposes, a specific three-dimensional, nonsymmetric, boundary value problem was studied. The problem is that of finding the steady-state temperature at any point inside the shielding of a simplified nuclear reactor. The reactor is modeled as a solid block one unit long, half a unit wide, and three-quarters of a unit tall with a spherical, high temperature, core placed in one corner (Fig. 1). The domain, Ω, then consists of the solid block minus the inside of the spherical core. The boundary is comprised of two disjoint parts: the surface of the block, Γ_b, and the surface of the core, Γ_c. The temperature of the outside surface of the reactor is defined to be 100 while the temperature of the inside sphere surface is set at a constant 1000. The differential equation governing the steady-state temperature distribution in the domain is the Laplacian:

$$\nabla^2\phi = \frac{\partial^2\phi}{\partial x^2} + \frac{\partial^2\phi}{\partial y^2} + \frac{\partial^2\phi}{\partial z^2} = 0 \tag{17}$$

where $\phi = \phi(x, y, z)$ is the absolute temperature at location (x, y, z). The problem statement is thus

$$\begin{aligned} \nabla^2(\phi) &= 0 \text{ in } \Omega; \\ \phi &= 100 \text{ on } \Gamma_b; \\ \phi &= 1000 \text{ on } \Gamma_c \end{aligned} \tag{18}$$

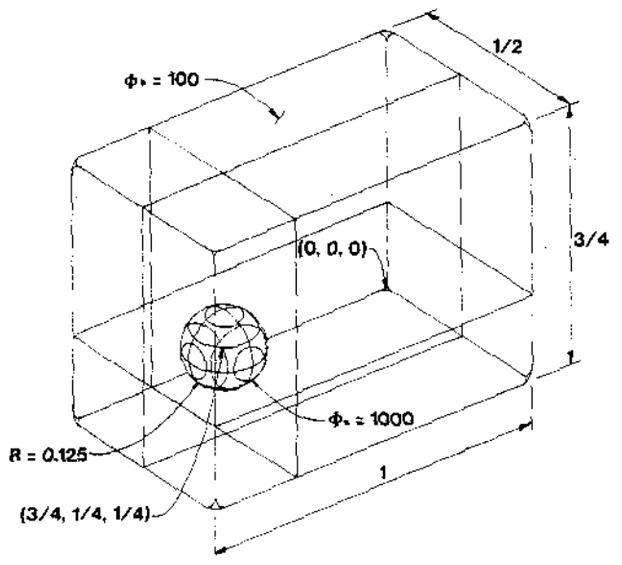

Fig. 1. Nuclear reactor problem definition (steady-state heat transport).

One corner of the box is located at $(0,0,0)$ and the opposite corner is $(1{\cdot}0, 0{\cdot}5, 0{\cdot}75)$. The center of the sphere is located at $(0{\cdot}74, 0{\cdot}25, 0{\cdot}25)$, and its radius is $0{\cdot}125$ units.

Trial functions

For the considered problem, all trial functions chosen satisfy the Laplacian everywhere on the domain and boundary. The trial functions considered are either harmonic polynomials, or the functions in eqn (19) with a singularity, not in the domain, which is like the singularity of a Green's function.

$$f(x,y,z) = \left(\frac{1}{(x-\hat{x})^2 + (y-\hat{y})^2 + (z-\hat{z})^2} \right)^{1/2} \qquad (19)$$

where $(\hat{x}, \hat{y}, \hat{z})$ is a point exterior to Ω and Γ.

The set of harmonic polynomial trial functions are readily extended by scalar multiplication and addition of other harmonic polynomials. The singular functions are dependent upon the choice of singularity point location,

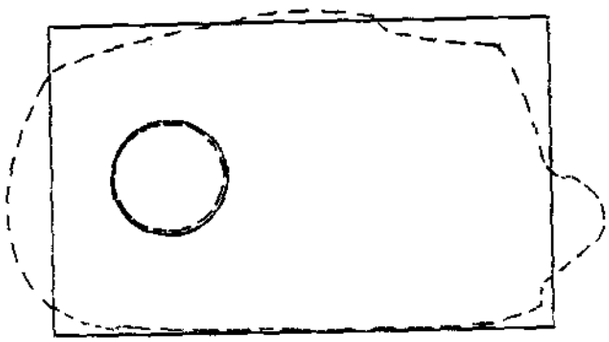

Fig. 2. Approximate boundary, $\hat{\Gamma}$, for horizontal $z = 0{\cdot}25$ slice. Twelve harmonic polynomials and 36 singular functions used.

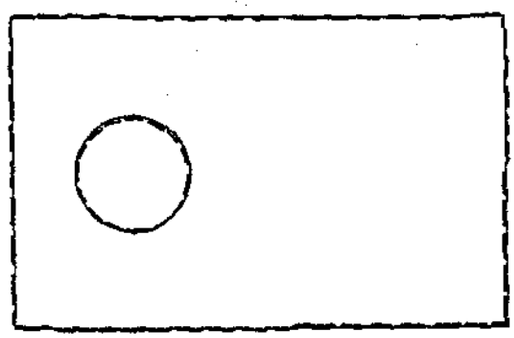

Fig. 3. Approximate boundary, $\hat{\Gamma}$, for horizontal $z = 0{\cdot}25$ slice. Sixteen harmonic polynomials and 84 singular functions used.

that surround the problem outer boundary or that lie inside the interior sphere. The sum of the several trial functions, each multiplied by some constant (to be determined) still retains the property of being harmonic throughout the problem domain. The trial function coefficients are then selected as described in the previous mathematical development.

Approximation accuracy is evaluated by plotting the approximate boundary $\hat{\Gamma}$ with respect to the true boundary Γ. In regions where $\hat{\Gamma}$ and Γ differ significantly, additional singular functions are added to the trial function set with singularities near that place, and harmonic polynomials are added as well. In this fashion, approximation error is reduced. It is recalled that for each approximation, the governing Laplace equation is satisfied exactly throughout Ω; however, there remains approximation error in satisfying the boundary conditions on Γ.

Constructing the approximate boundary, $\hat{\Gamma}$

For each trial approximation, the approximate boundary $\hat{\Gamma}$ is developed as a set of two-dimensional slices of $\Omega \cup \Gamma$. A slice of key interest is the horizontal one located at vertical coordinate $z = 0{\cdot}25$, which corresponds to the equator of the spherical core; it was

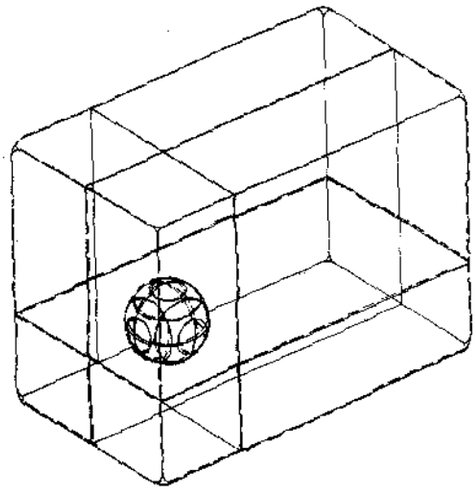

Fig. 4. Approximate boundary $\hat{\Gamma}$ for approximation of Fig. 3.

discovered that the $z = 0{\cdot}25$ horizontal slice generally showed the greatest discrepancy between $\hat{\Gamma}$ and Γ. (Similar slices in the x–z and y–z directions were also considered).

For a selected set of trial functions, the model $\hat{\phi}_m$ is developed using the previous generalized Fourier series construction. The $\hat{\phi}_m(x, y, z)$ is used to evaluate the location of the isotherm $\hat{\phi}_m(x, y, z = 0{\cdot}25) = 1000$ and also the location of the isotherm $\hat{\phi}_m(x, y, z = 0{\cdot}25) = 100$; the resulting $\hat{\phi}_m$ isotherms are associated to boundary contours Γ_b and Γ_c, respectively.

As additional trial functions are added to the set, $\hat{\Gamma}$ was approached geometrically. Figures 2 and 3 demonstrate $\hat{\Gamma}$ plots on the $z = 0{\cdot}25$ horizontal slice through $\Omega \cup \Gamma$ for two sets of trial functions. It is noted that in Fig. 3, the second set of trial functions is based on the departures between Γ and $\hat{\Gamma}$ from Fig. 2. Figure 4 shows several $\hat{\Gamma}$ plots for horizontal slices through $\Omega \cup \Gamma$, using the trial function set of Fig. 3. From Fig. 4, $\hat{\Gamma}$ may be sufficiently close to Γ to suggest that the $\hat{\phi}_m$ function is adequate as an approximation of the boundary value problem. If $\hat{\Gamma}$ is acceptable as being the 'true' problem geometric shape, then $\hat{\phi}_m$ is the exact solution to the 'new' boundary value problem.

CONCLUSIONS

In this paper, the best approximation method is applied to three-dimensional steady-state heat transport problems. Additionally, the approximate boundary technique is used to demonstrate approximation error in satisfying the problem auxiliary conditions. Because of the approximate boundary approach, numerical approximation error is perhaps more easily visualized than other, more conventional, methods of evaluating the approximate error.

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