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A meshless singular boundary method for three-dimensional inverse heat conduction problems in general anisotropic media

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ABSTRACT

The singular boundary method (SBM) is a relatively new meshless boundary collocation method for the numerical solution of certain elliptic boundary value problems. The method, based on the notion of the boundary element method (BEM) and method of fundamental solutions (MFS), fully inherits the merits of both and in the meantime possessing its unique advantages. Due to the boundary-only discretizations and its semi-analytical nature, the method can be viewed as an ideal candidate for the solution of inverse problems. In this study, we document the first attempt to apply the SBM, together with several regularization techniques, for the solution of inverse heat conduction problems in three-dimensional (3D) anisotropic media. Four benchmark numerical examples are well-studied which indicate that the proposed scheme is accurate, computationally efficient and numerically stable for the solution of 3D inverse problems with various levels of noisy input data.

1. Introduction

The finite element method (FEM) has long been a dominant numerical technique in the simulation of real-world engineering applications. However, this method requires the task of meshing the whole domain which can be arduous, time-consuming and computationally expensive for certain classes of problems. So the FEM, despite the generality of its application in engineering problems, is not free of drawbacks. As an alternative approach, the boundary element method (BEM) has long been touted to avoid such shortcomings due to the boundary-only discretizations and its semi-analytical nature [1]. During the past two decades, the BEM has rapidly improved, and is nowadays considered as a competing method to the FEM. However, it is well-known that the BEM cannot be used for problems whose fundamental solution is either not known or cannot be determined. Such are, for example, problems described by differential equations with variable coefficients. The method is also not applicable to non-linear problems for which the principle of superposition does not hold. In this case, a BEM model procedures domain integrals that can be computed by discretizing the domain, but this, of course, spoils the pure boundary character of the method. In addition, despite the fact that the BEM requires only meshing on the boundary, surface meshing in a 3D object with complicated geometry is still a nontrivial task. Thus, over the past decade, some considerable effort was devoted to circumventing or greatly eliminating the need for meshing. This led to the development of meshless or meshfree methods which require neither domain nor boundary meshing. Some interesting remarks of the meshless methods and their engineering applications may be found in the survey papers [2–4].

The singular boundary method (SBM) [5] is a relatively new method for the numerical solution of boundary/initial value problems governed by certain partial differential equations. The method belongs to the family of meshless boundary collocation methods and involves a coupling between the regularized indirect boundary element method (BEM) and the method of fundamental solutions (MFS) [6–8]. The main idea is to fully inherit the dimensionality and stability advantages of the former and the meshless and integration-free attributes of the later. The advantages that the SBM has over the more classical domain or boundary discretization methods can be summarized as follows. First of all, it is a boundary-type method which means that it shares the same advantages of the BEM has over domain discretization methods. Secondly, it is meshless and does not require the task of domain and/or boundary meshing which can be arduous, time-consuming and computationally expensive for problems in complex geometries and higher dimensions. Thirdly, it does not involve costly integrations which could

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be otherwise troublesome as in the case, for example, the BEM-based methods. Finally, the method sidesteps the perplexing *fictitious boundary issue* [9–11] associated with the traditional MFS while inheriting the merits of the latter of being truly meshless, mathematically simple and easy-to-program. These features make the method particularly attractive for the solution of problems in which the boundary is of major importance or requires special attention. However, as its current stage of development, the SBM also exhibits several disadvantages, the most important of which are: (1) similar to the BEM, the SBM cannot be used for problems whose fundamental solution is not known; and (2) the SBM produces dense and unsymmetrical coefficient matrix, therefore, the method may be arduous, time consuming, and computationally expensive for the solution of large-scale problems. During the past few years, intense research has been conducted in an effort to overcome the aforementioned disadvantages.

Prior to this study, the SBM has been successfully tried for 2D problems in potential theory [12] and linear elasticity [5]. Very recently, the method has also been extended to solve 3D problems in potential theory [13]. These problems are known as well-posed direct problems in which the Dirichlet or Neumann data on the whole boundary are known. In contrast, in inverse problems, one or more of the data describing the direct problem is missing, due to technical difficulties associated with data acquisition. To fully determine the process, additional data must be supplied, either other boundary conditions on the same accessible part of boundary or measurements at some internal points in the domain. A formal mathematical model of an inverse problem can be derived with relative ease. However, the process of solving such problems is extremely difficult and the so-called exact solution practically does not exist. The inverse problems are also difficult to solve numerically due to the fact that they are ill-posed in the sense that small errors in measured data may lead arbitrarily large changes in the numerical solution [14,15]. Since the measured data are usually observed only on a part of the boundary, the boundary-type methods, such as the BEM and MFS, have an edge over domain-type methods for the numerical solution of such problems. Some interesting surveys of the BEM and MFS on the inverse and ill-posed problems can be found in Refs. [16–19].

Motivated by the rapidly growing interest in the area, our aim in this article is to document the first attempt to extend the SBM for the solution of inverse heat conduction problems in 3D anisotropic media. Heat conduction in these non-isotropic materials has numerous important applications in various branches of sciences and engineering [20,21]. Since the matrix arising from the SBM discretization for inverse problems is severely ill-conditioned, a regularized solution is obtained here by employing some regularization strategies, namely the truncated singular value decomposition (TSVD) [22] and Tikhonov regularization technique [23], whilst the optimal regularization parameter is determined by the *L*-curve criterion.

A brief outline of the rest of this paper is as follows. Section 2 introduces the mathematical formulation of Cauchy problems in general 3D anisotropic medium. The SBM formulation and its numerical implementation are reviewed in Section 3. Followed in Section 4, the SBM formulations are combined with the aforementioned regularization techniques to solve the ill-conditioned system of algebraic equations. Four benchmark test problems on general 3D anisotropic media with both smooth and piecewise smooth geometries are examined in Section 5. Finally, the conclusions and remarks are provided in Section 6.

2. Mathematical formulation for 3D steady-state heat conduction problems

Consider a 3D anisotropic medium in an open bounded domain Ω, and assume that Ω is bounded by a surface $\partial\Omega = \Gamma$ which may consist of several components, each being sufficiently smooth in the sense of Liapunov. We also assume that the boundary consists of two parts, $\Gamma = \Gamma_1 \cup \Gamma_2$, where $\Gamma_1, \Gamma_2 \neq \emptyset$ and $\Gamma_1 \cap \Gamma_2 = \emptyset$. In this study, we refer to anisotropic steady heat conduction applications in the absence of inner heat sources. Hence the function $u(\boldsymbol{x})$, which denotes the temperature distribution in Ω, satisfies the equation

$$k_{ij}\frac{\partial^2 u(\boldsymbol{x})}{\partial x_i \partial x_j} = 0, \quad \boldsymbol{x} \in \Omega, \quad (i,j = 1,2,3) \tag{1}$$

subject to the following boundary conditions

$$u(\boldsymbol{x}) = \bar{u}(\boldsymbol{x}) \quad \text{for } \boldsymbol{x} \in \Gamma_1, \tag{2}$$

$$q(\boldsymbol{x}) = \frac{\partial u}{\partial \boldsymbol{n}}(\boldsymbol{x}) = \bar{q}(\boldsymbol{x}) \quad \text{for } \boldsymbol{x} \in \Gamma_1, \tag{3}$$

where $(k_{ij})_{i,j=1,2,3}$ are the thermal conductivity tensor, which is assumed to be symmetric and positive-definite so that the partial differential Eq. (1) is elliptic, $\boldsymbol{n}$ denotes the outward normal, the overline quantities $\bar{u}(\boldsymbol{x})$ and $\bar{q}(\boldsymbol{x})$ indicate the given values on the boundary. The customary standard Einstein notation for summation over repeated subscripts is employed. In the above formulation of the boundary conditions (2) and (3), it can be seen that the boundary Γ_1 is over-specified by prescribing both the temperature and the heat flux, whilst the remaining boundary Γ_2 is under-specified since both the temperature and the heat flux are unknown and have to be determined.

From thermodynamic considerations and Onsager's reciprocity relation, the conductivity tensor $(k_{ij})_{i,j=1,2,3}$ must satisfy

$$k_{11}k_{33} - k_{13}^2 > 0, \quad k_{11}k_{22} - k_{12}^2 > 0, \quad k_{22}k_{33} - k_{23}^2 > 0. \tag{4}$$

The heat flux vector in an anisotropic potential problem in Ω is defined as

$$h_i(\boldsymbol{x}) = k_{ij}u_{,j}(\boldsymbol{x}) \tag{5}$$

and the normal heat flux through the boundary Γ is given by

$$q(\boldsymbol{x}) = n_i(x)h_i(\boldsymbol{x}), \tag{6}$$

where $u_{,j}(\boldsymbol{x}) = \frac{\partial u(\boldsymbol{x})}{\partial x_j}$ represents the derivatives of the temperature $u(\boldsymbol{x})$ with respect to x_j, and $n_j(\boldsymbol{x})$ is the directional cosine of the unit outward normal vector at the boundary point $\boldsymbol{x}$.

In the traditional MFS [24], the solution $u(\boldsymbol{x})$ and $q(\boldsymbol{x}) = \frac{\partial u(\boldsymbol{x})}{\partial \boldsymbol{n}_x}$ can be approximated by a linear combination of fundamental solutions with respect to different source points s^j as follows

$$u(\boldsymbol{x}^i) = \sum_{j=1}^{N=N_1+N_2} \alpha^j G(\boldsymbol{x}^i, \boldsymbol{s}^j), \tag{7}$$

$$q(\boldsymbol{x}^i) = \frac{\partial u(\boldsymbol{x}^i)}{\partial \boldsymbol{n}_{x^i}} = \sum_{j=1}^{N=N_1+N_2} \alpha^j \frac{\partial G(\boldsymbol{x}^i, \boldsymbol{s}^j)}{\partial \boldsymbol{n}_{x^i}}, \tag{8}$$

where $\boldsymbol{x}^i \in \bar{\Omega} = \Omega \cup \partial\Omega$ is the ith collocation point, s^j is the jth source point, α^j denotes the jth unknown coefficient of the distributed source at s^j, the indices N_1 and N_2 are numbers of the boundary nodes on Γ_1 and Γ_2, respectively, and

$$G(\boldsymbol{x}^i, \boldsymbol{s}^j) = \frac{1}{4\pi\sqrt{|k_{ij}|}\, r(\boldsymbol{x}^i, \boldsymbol{s}^j)}, \quad \boldsymbol{x}^i, \boldsymbol{s}^j \in R^3 \tag{9}$$

is the fundamental solutions [25] for 3D anisotropic heat conduction problems in which $|k_{ij}|$ denotes the determinant of k_{ij}. Employing indicial notation for the coordinates of points x and s, i.e. (x_1, x_2, x_3) and (s_1, s_2, s_3), respectively, the distance function $r(\boldsymbol{x}, \boldsymbol{s})$ in the above Eq. (9) can be expressed as

$$r(\boldsymbol{x}, \boldsymbol{s}) = \sqrt{t_{ij}(x_i - s_i)(x_j - s_j)}, \quad (i,j = 1,2,3), \tag{10}$$