Singular Boundary Method for Heat Conduction in Layered Materials

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Abstract: In this paper, we investigate the application of the singular boundary method (SBM) to two-dimensional problems of steady-state heat conduction in isotropic bimaterials. A domain decomposition technique is employed where the bimaterial is decomposed into two subdomains, and in each subdomain, the solution is approximated separately by an SBM-type expansion. The proposed method is tested and compared on several benchmark test problems, and its relative merits over the other boundary discretization methods, such as the method of fundamental solution (MFS) and the boundary element method (BEM), are also discussed.

Keywords: Singular boundary method, origin intensity factor, heat conduction, bimaterials, meshless.

1 Introduction

During machining processes, heat is a source that strongly influences the tool performance, such as tool wear, tool life, surface quality as well as process quality. The layers of material provide a barrier for the intensive heat flow from the contact area into the substrate material. Thus, a clear understanding of the temperature distribution in layered materials is very useful and important [Atluri (2005); Atluri, Liu, and Han (2006); Chang, Liu, and Chang (2010); Chen and Liu (2001)].

The method of fundamental solutions (MFS) [Karageorghis (1992); Fairweather and Karageorghis (1998); Chen, Golberg, and Hon (1998)] is a successful technique for the solution of some elliptic boundary value problems in engineering applications. It is applicable when a fundamental solution of the operator of the governing equation is known. The solution of the problem is approximated by a linear combination of fundamental solutions expressed in terms of sources located outside the
domain of the problem. Despite many years of great effort, the determination of the fictitious boundary remains largely a trial-error approach. Some of its recent applications to coating systems can be found in Refs. [Berger and Karageorghis (1999, 2001)]. All of these studies show that the optimal distance between the real boundary and the fictitious boundary is critical to accurately evaluate the temperature or stress fields in layered materials.

In recent years, tremendous effort has been made to derive sophisticated computational techniques to overcome the above-mentioned barriers in the MFS. The proposed methods include, but are not limited to, the boundary knot method (BKM) [Chen and Hon (2003); Chen and Tanaka (2002)], the regularized meshless method (RMM) [Chen, Kao, Chen, and Wu (2009); Young, Chen, and Lee (2005)], the modified method of fundamental solution (MMFS) [Sarler (2009)], and the boundary distributed source (BDS) method [Liu (2010)]. The above methods have been reviewed in Refs. [Chen, Fu, and Wei (2009); Liu (2010)]. In a more recent study, Chen and his collaborators [Chen (2009); Chen and Wang (2010)] proposed a new boundary-type meshless method, namely singular boundary method (SBM), in which a new fundamental concept is the origin intensity factor (OIF). It is assumed that the singular term of the fundamental solution upon the coincidence of the source and collocation points can be isolated and exits in the strong-form collocation methods for the well-posed problems. And then the OIF is calculated by an inverse interpolation technique (IIT), without the need of using a fictitious boundary or any integration. This method is truly meshless and has been successfully applied to interior and exterior problems of Laplace and Helmholtz equations [Chen and Fu (2009); Chen, Fu, and Wei (2009)].

In this paper, we first extend the SBM to problems of steady-state heat conduction in isotropic bimaterials. A domain decomposition technique, namely the multi-domain singular boundary method (MD-SBM), is proposed. The bimaterial is decomposed into two subdomains, and in each subdomain, the solution is approximated separately by an SBM-type expansion. On the subdomain interface, we impose the continuity condition of the temperatures and the fluxes.

A brief outline of this research is as follows. In Section 2, we describe the SBM in the solution of isotropic problems in a single material. In Section 3, we present the MD-SBM for heat conduction in bimaterial problems, followed by Section 4 where the accuracy and stability of the proposed strategy are tested to the two benchmark bimaterial problems. The MD-SBM solutions are compared with the results obtained by using the MFS, the BEM, and exact solutions. Finally, the paper is summarized in Section 5.
2 The SBM for heat conduction in a single material

We consider the generalized Laplace equation for steady-state heat conduction in an isotropic solid

$$\nabla^2 u(x) = 0, \quad x \in \Omega$$  \hspace{1cm} (1)

subjected to the boundary conditions

$$Bu(x) = f(x), \quad x \in \partial \Omega$$  \hspace{1cm} (2)

where $\nabla^2$ denotes the Laplacian operator, $\Omega$ is a bounded domain in $R^2$ with boundary $\partial \Omega$, which we shall assume to be piecewise smooth. The operator $B$ can be selected to specify Dirichlet, Neumann or Robin boundary conditions. The fundamental solution of Eq. (1) is

$$u^*(x_i, x_j) = -\frac{1}{2\pi} \ln \|x_i - x_j\|_2$$  \hspace{1cm} (3)

Similar to the MFS, the SBM also uses the fundamental solution as the kernel function of the approximation. In contrast to the MFS, the collocation and source points of the SBM are selected as the same set of boundary nodes which are placed on the physical boundary instead of on the fictitious boundary. In the SBM, the interpolation formula is given by [Chen and Wang (2010)]

$$u(x_i) = \sum_{j=1, j \neq i}^{N} \alpha_j u^*(x_i, x_j) + \alpha_i q_{ii}, \quad i = 1, 2, ..., N$$  \hspace{1cm} (4)

where $x_i$ is the $i$th collocation point, $x_j$ is the $j$th source point located on real boundary, $\alpha_j$ is the $j$th unknown intensity of the distributed source at $x_j$, $q_{ii}$ is defined as the origin intensity factor (OIF). The fundamental assumption of the SBM is the existence of the OIF upon the singularity of the coincident source-collocation nodes for mathematically well-posed problems. Our findings are that OIF does exist and its value is of a finite value, depending on the distribution of discrete boundary nodes and respective boundary conditions.

The essential difference between the variety of existing boundary-type meshless methods is how to evaluate the origin intensity factor. The BKM [Chen and Tanaka (2002); Chen and Hon (2003); Chen, Fu, and Qin (2009); Wang, Ling, and Chen (2009)] uses the nonsingular general solutions instead of using the singular fundamental solutions to avoid the singularity of the origin intensity factor. The RMM [Young, Chen, and Lee (2005); Young, Chen, Chen, and Kao (2007)] employs the
subtracting and adding-back techniques in the BEM, based on the fact that the MFS and the indirect boundary integral formulation are similar in nature. The MMFS [Sarler (2009)] determines the diagonal terms by the integration of the fundamental solution on line segments formed by surrounding points, and a constant sample solution is employed to determine the diagonal coefficients of the derivatives of the fundamental solution. In the BDS approach [Liu (2010)], the singular fundamental solution is integrated over small surrounding line or surface covering the source points so that the OIF can analytically be evaluated. Unlike the above-mentioned methods, the SBM uses an inverse interpolation technique to evaluate the singular diagonal elements in its discretization matrix under the coincidence of source and collocation points on the physical boundary, without using any element or integration concept.

The matrix form of Eq. (4) can be written as

\[
\{ q_{ij} \} \{ \alpha_j \} = \{ u(x_i) \}
\] (5)

where \( q_{ij} = u^*(x_i, x_j) \). We can observe that \( q_{ii} \) are the diagonal elements of the discretization matrix \( Q = \{ q_{ij} \} \). By collocating \( N \) source points on the physical boundary to satisfy the boundary condition (2), we obtain the following discretization algebraic equations:

\[
\{ q_{ij} \} \{ \alpha_j \} = \{ f(x_i) \}
\] (6)

Obviously, we can not simply use the fundamental solutions to calculate \( q_{ii} \). Instead, the SBM uses an inverse interpolation technique to determine the diagonal elements \( q_{ii} \) in Eq. (6). In this strategy, we first place a cluster of sample points \( x_k \) inside the physical domain. Then we choose a simple particular solution as the sample solution, e.g., \( u(x, y) = x + y \) in Laplace equation case. Using the interpolation formula (4), we can get

\[
\{ b_{kj} \} \{ s_j \} = \{ x_k + y_k \}
\] (7)

where \( b_{kj} = u^*(x_k, x_j) \). Thus the corresponding influence coefficients \( s_j \) can be evaluated. Replacing the computational collocation points \( x_k \) with the boundary collocation point \( x_i \), we have the following algebraic equations

\[
\{ q_{ij} \} \{ s_j \} = \{ x_i + y_i \}
\] (8)

It is noted that only the source intensity factors \( q_{ii} \) are unknown in the above equation, hence the source intensity factors can be calculated by using the following
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formulation:

\[
q_{ii} = \frac{1}{s_i} (x_i + y_i - \sum_{j=1, i \neq j}^{N} q_{ij}s_j), \quad i = 1, 2, \ldots, N
\]  

(9)

Note that the source intensity factors only depend on the distribution of the source points and boundary conditions. Theoretically speaking, the source intensity factors remain unchanged under different sample solutions with the inverse interpolation technique.

3 The SBM formulation for bimaterial problems

In the machining industry, the layers of the material protect the tool against adhesion diffusion, intensive abrasive wear and also provide a barrier for the intensive heat flow from the contact area into the substrate material. One way to model the layered systems is to use domain decomposition technique (DDT). The basic idea behind the DDT is that the whole domain of concern is broken up into separated subdomains and the final system of equations is constituted by assembling algebraic equations discretized in each subdomain, based on the compatibility of temperatures and normal fluxes at adjacent common interface nodes. Since the DDT can deal with multi-material problems and results in algebraic equations with a blocked sparse coefficient matrix, it has been extensively used in past decades to solve various engineering problems [Gao, and Guo, and Zhang (2007)].

![Figure 1: Boundary discretization of the bimaterial](image)

A generic two-domains problem is illustrated in Fig. 1 where the entire domain is decomposed into the two homogenous and isotropic subdomains \(\Omega^I\) and \(\Omega^II\). The
exterior boundary of subdomain $\Omega^I$ is $\Gamma^I$ and that of subdomain $\Omega^{II}$ is $\Gamma^{II}$. The contact interface between the two subdomains is denoted by $\Gamma^c$. The coefficients of heat conductivity of these two subdomains are represented by $k^I$ and $k^{II}$.

The bimaterial problems under consideration in this study will be solved via a multi-domain singular boundary method (MD-SBM) developed for steady-state heat conduction problems. The bimaterial is decomposed into two subdomains, and in each subdomain, the solution is approximated by a SBM-type expansion. In $\Omega^I$, the solution is approximated by

$$u^I(x^I_i) = \sum_{j=1,j\neq i}^{N} \alpha^I_j u^*(x^I_i,x^I_j) + \alpha^I_i q^I_{ii} x^I_i \in \bar{\Omega}^I, \ x^I_j \in \partial \Omega^I$$

and, in $\Omega^{II}$, the solution is approximated by

$$u^{II}(x^{II}_i) = \sum_{j=1,j\neq i}^{N} \alpha^{II}_j u^*(x^{II}_i,x^{II}_j) + \alpha^{II}_i q^{II}_{ii} x^{II}_i \in \bar{\Omega}^{II}, \ x^{II}_j \in \partial \Omega^{II}$$

in which the source intensity factors $q^I_{ii}$ and $q^{II}_{ii}$ can be calculated by using the inverse interpolation technique stated in Section 2.

First, the exterior boundary $\Gamma^I$ of subdomain $\Omega^I$, as shown in Fig. 1, is analyzed. One can get the following discretized algebraic equations

$$[G^I] \left( \begin{array}{c} \{ \alpha^I \} \\
\{ \alpha^I_c \} \end{array} \right) = \{ U^I \} , \quad [G^I_c] \left( \begin{array}{c} \{ \alpha^I \} \\
\{ \alpha^I_c \} \end{array} \right) = \{ U^I_c \}$$

$$[H^I] \left( \begin{array}{c} \{ \alpha^I \} \\
\{ \alpha^I_c \} \end{array} \right) = \{ Q^I \} , \quad [H^I_c] \left( \begin{array}{c} \{ \alpha^I \} \\
\{ \alpha^I_c \} \end{array} \right) = \{ Q^I_c \}$$

where $U^I_c$ and $Q^I_c$ are the interface temperature and normal derivative of temperature of the subdomain $\Omega^I$ on the interface $\Gamma^c$, $U^I$ and $Q^I$ the temperature and normal derivative of temperature of the subdomain $\Omega^I$ on the remaining surfaces. $\alpha^I$ and $\alpha^I_c$ denote the unknown coefficients on $\Gamma^I$ and $\Gamma^c$ of the subdomain $\Omega^I$, respectively. $G^I, G^I_c, H^I$ and $H^I_c$ are the corresponding coefficient matrix.

Similarly, for the subdomain $\Omega^{II}$, we have

$$[G^{II}] \left( \begin{array}{c} \{ \alpha^{II} \} \\
\{ \alpha^{II}_c \} \end{array} \right) = \{ U^{II} \} , \quad [G^{II}_c] \left( \begin{array}{c} \{ \alpha^{II} \} \\
\{ \alpha^{II}_c \} \end{array} \right) = \{ U^{II}_c \}$$

$$[H^{II}] \left( \begin{array}{c} \{ \alpha^{II} \} \\
\{ \alpha^{II}_c \} \end{array} \right) = \{ Q^{II} \} , \quad [H^{II}_c] \left( \begin{array}{c} \{ \alpha^{II} \} \\
\{ \alpha^{II}_c \} \end{array} \right) = \{ Q^{II}_c \}$$
For a well-posed boundary value problem, either $U$ or $Q$ are known at each nodal point on the physical boundaries. However, along the interface $\Gamma_c$, both $U$ and $Q$ are unknowns. To solve the problem numerically, there will be the same number of algebraic equations as the unknowns. Therefore, the following continuity conditions at the interface must be considered:

Continuity of temperature on $\Gamma_c$:

$$U^I_c = U^II_c$$  \hspace{1cm} (16)

Continuity of normal flux on $\Gamma_c$:

$$k^I Q^I_c = -k^II Q^II_c$$  \hspace{1cm} (17)

In order to illustrate the SBM-based procedures in a more clear fashion without loss of generality, we here suppose that the temperature boundary conditions are prescribed on $\Gamma^I$ and $\Gamma^II$. According to the equilibrium and compatibility conditions (14) and (15) at the interface, discretized algebraic equations (12) and (13) can be coupled as:

$$
\begin{bmatrix}
G^I \\
G^I_c \\
H^I \\
0
\end{bmatrix}
- 
\frac{k^II}{k^I}
\begin{bmatrix}
G^II_c \\
H^II_c
\end{bmatrix}
= 
\begin{bmatrix}
\{U^I\} \\
\{0\} \\
\{0\} \\
\{U^II\}
\end{bmatrix}
$$  \hspace{1cm} (18)

For multi-coating problems, more equations will be added to the above equations (16) in a similar way. The system of discretized algebraic equations still needs to be reordered according to the prescribed temperature and normal flux boundary conditions. The system of equations (16) can simultaneously be solved for the boundary and interface unknowns. Once the boundary unknowns are solved, Eqs. (10) and (11) can be integrated to obtain the temperature distributions at any point inside each subdomain.

4 Numerical examples and discussions

To verify the MD-SBM scheme developed in the foregoing section, the two benchmark bimaterial problems are examined in which the SBM solutions are compared with the conventional MFS and the BEM. The root mean square (relative) error is defined by

$$\text{Relative Error} = \left[ \frac{1}{M} \sum_{k=1}^{M} \left( \frac{I_{\text{numerical}} - I_{\text{exact}}}{I_{\text{exact}}} \right)^2 \right]^{1/2}$$  \hspace{1cm} (19)
where $I_{\text{numerical}}$ represents numerical result and $I_{\text{exact}}$ is analytic solution of the considered problem.

Figure 2: A cylinder coating on a shaft

Figure 3: Relative error curves of the computed temperatures, respectively, by using the SBM, the BEM and the MFS
4.1 Test problem 1: A cylinder coating on a shaft

As depicted in Fig.2, a coating with uniform thickness on a shaft is considered. The domain $\Omega^I$ is the coating with the inner and outer radii $r_2 = 2$ and $r_3 = 3$, and the domain $\Omega^{II}$ is the substrate with the inner radius $r_1 = 1$. The Dirichlet boundary condition is imposed on the edge of the coating system, using the following analytical solution

$$u(r, \theta) = r^6 \cos(6\theta)$$

In this example, it is assumed that the shaft and the coating are made of the same material and share the same heat conductivity. Actually, in this special case, the temperature distributions in bimaterial are in fact that of the single material. The MD-SBM is applied here simply to obtain these temperature distributions inside this single material domain, in order to verify the validity of the MD-SBM solutions when analytical solutions are not available for different coating/shaft combinations.

The number of boundary nodes used varies from 150 to 1800. A number of $M = 260$ field points are selected inside the domain along the circle with radius $r = 1.5$ and center at the origin, and the solutions at these field points are computed and compared with the analytical solution. The BEM and the traditional MFS is also used for the purpose of comparison. For the MFS solutions, the fictitious boundary is chosen to be a circle with radius $r = 4$ and center at the origin, and the source points are uniformly distributed on this fictitious boundary. The BEM solutions are obtained by using the indirect boundary integral equations with quadratic discontinuous boundary elements, because in most engineering applications, the quadratic element is good enough to approximate curvilinear boundary with sufficient accuracy. It is stressed that the number of boundary nodes is the same in the SBM, the BEM and the MFS.

Figs. 3 and 4 display the relative error curves of the computed temperatures $u$ and fluxes $\partial u / \partial x_1$ at the field points inside the domain, respectively, by using the SBM and compared with the results using the BEM and the MFS. As shown in Figs. 3 and 4, the SBM and the other two numerical methods yield highly accurate temperature and flux results when compared with analytical solutions. In fact, as demonstrated here, the SBM can perform as equally well as the BEM. It is also noted that the MFS can obtain very accurate solution if the artificial boundary is carefully chosen as in this case shown in Figs. 3 and 4. But in many real-world applications, the determining of good artificial boundary is a difficult task.
The number of boundary nodes used varies from 150 to 1800. A number of $260M = 2M$ field points are selected inside the domain along the circle with radius $1.5r = 1.5r$ and center at the origin, and the solutions at these field points are computed and compared with the analytical solution. The BEM and the traditional MFS is also used for the purpose of comparison. For the MFS solutions, the fictitious boundary is chosen to be a circle with radius $4r = 4r$ and center at the origin, and the source points are uniformly distributed on this fictitious boundary. The BEM solutions are obtained by using the indirect boundary integral equations with quadratic discontinuous boundary elements, because in most engineering applications, the quadratic element is good enough to approximate curvilinear boundary with sufficient accuracy. It is stressed that the number of boundary nodes is the same in the SBM, the BEM and the MFS.

![Figure 4: Relative error curves of the computed fluxes, respectively, by using the SBM, the BEM and the MFS](image)

Figure 4: Relative error curves of the computed fluxes, respectively, by using the SBM, the BEM and the MFS

$T_I = 3x_1^2 - 3x_2^2 + 2x_1x_2 + x_1 + 6x_2$

$T_2 = 3x_1^2 - 3x_2^2 + x_1x_2 + 2x_1 + 6x_2$

![Figure 5: Configuration of heat conduction for layered rectangle](image)

Figure 5: Configuration of heat conduction for layered rectangle

### 4.2 Test problem 2: A coating on a rectangle

In the second test case, we construct a configuration that is closer to a real-world machining process, as shown in Fig. 5, a $2 \times 1 \text{ m}^2$ rectangle with a coating of thickness $h = 0.5$. The boundary conditions are specified in Fig. 5. In this example,
the mediums of domain $\Omega^I$ and $\Omega^{II}$ are assumed to have heat conductivities of $K_1 = 1 \text{ W/mk}$ and $K_2 = 2 \text{ W/mk}$, respectively. The domain $\Omega^I$ is considered the coating layer with thickness $h = 0.5$ and $\Omega^{II}$ is its substrate counterpart. The number of boundary nodes used varies from 40 to 520. $M = 200$ field points are selected inside the domain along the lines $y = 0.5$ and $y = 1.25$ with $0.2 \leq x \leq 1.8$, and the solutions at these field points are computed and compared with the analytical solutions. The BEM and the MFS is also used for solving this problem. For the MFS solutions, the fictitious boundary is chosen to be a rectangle $(-1,3) \times (-1,2.5)$, and the source points are uniformly distributed on this fictitious boundary. The BEM solutions are obtained by using the indirect boundary integral equations with linear discontinuous boundary elements. It is worth noting that linear boundary element is adequate in this case because it can exactly represent straight line boundary. Also, it is stressed that the number of boundary nodes is the same in the SBM, the BEM and the MFS.

Figs. 6 and 7 display the relative error curves of the computed temperatures $u$ and fluxes $\partial u / \partial x_1$ at the field points inside the domain, respectively, by using the SBM, the BEM and the MFS. The SBM results have better accuracy than the BEM results, i.e., when using 520 boundary nodes, the SBM is more accurate than the BEM by about three orders of magnitude. Again, we can observe that the MFS can be used to obtain very accurate solution if the artificial boundary is carefully chosen. But in many real-world applications, the determining of good artificial boundary is a
Figure 6: Relative error curves of the computed temperatures, respectively, by using the SBM, the BEM and the MFS

Figure 7: Relative error curves of the computed fluxes, respectively, by using the SBM, the BEM and the MFS

difficult task.

5 Conclusions

This study demonstrates the applicability of the SBM to bimaterial problems of steady-state heat conduction. A domain decomposition technique, termed the multi-domain singular boundary method, is developed. The bimaterial is decomposed into two subdomains, and in each subdomain, the solution is approximated separately by an SBM-type expansion. On the subdomain interface, the continuity of the temperatures and the corresponding fluxes is imposed. Numerical experiments indicate that the proposed MD-SBM technique agrees pretty well with the MFS and the BEM in terms of efficiency and accuracy. The proposed SBM scheme for bimatirals also offers great promise for the analysis and modeling of the other industrial problems, such as multi-layered coating systems, internal stresses in thin-coated materials. Some work along this line is underway.

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