Shape optimizations of inhomogeneities of two dimensional (2D) and three dimensional (3D) steady state heat conduction problems by the boundary element method

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ABSTRACT

The shape optimizations of inhomogeneities for 2D and 3D steady state heat conductions in an infinite medium are respectively studied by the boundary element method (BEM). Interest in the shape optimization by the BEM is mainly due to its high computation accuracy and simplicity in meshing. The boundary integral equations and the heat energy formulations in this paper only contain the temperature on each inhomogeneity–matrix interface. The heat energy increment in the inhomogeneous medium is taken as the objective function. The method of moving asymptotes (MMA) is adopted to carry out numerical implementation of the shape optimizations of 2D and 3D inhomogeneities.

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1. Introduction

The optimization of material microstructures is of great interest to designers and researchers. The reason is in the fact that the geometrical shape and physical properties of material microstructures have important influence on the whole behavior of composite structures. A lot of literature is devoted to optimizing material microstructures with various objectives, e.g. maximum stiffness and conductivity [1], extreme thermal conductivity [2] and maximum permeability [3]. Kachanov and Sevostianov [4] showed that the effective properties of composite system are more sensitive to geometrical shapes of inhomogeneities rather than to elastic interactions among inhomogeneities. Shenfeld et al. [5] investigated optimal shape of an inhomogeneity in a two-phase elastic composite using the finite element method (FEM). Their method assumes that the inhomogeneity has a doubly symmetric shape which is only suitable for remote inhomogeneities from each other. The whole composite domain needs to be discretized into a lot of finite elements, especially more fine finite elements have to be used near the inhomogeneity–matrix interface for obtaining more accurate numerical results. Prochazka [6] presented a BEM optimization procedure based on homogenization technique, in which a special constraint was put into the formulation of optimal shape of a hole by Lagrangian multiplier. Compared with the FEM, the BEM has the particular advantage in the shape optimization of elastic or heat conduction inhomogeneities since the shape optimization is only limited to a moving boundary or interface problem [7–12].

The purpose of this paper is devoted to the study of the shape optimizations of inhomogeneities of 2D and 3D steady state heat conduction problems, in which the minimum heat energy increments of various inhomogeneous media under the heat flux are considered to be the objective functions. The boundary integral equations and the heat energy calculation formulations in this research only contain the temperature on each inhomogeneity–matrix interface. The constrains in the optimization process are taken as the areas (2D)/volumes (3D) of the inhomogeneities. The radial distance of each point from its center on each 2D inhomogeneity is considered as the design variable. For 3D inhomogeneous problems, three semi-major axes for each ellipsoidal inhomogeneity are respectively taken as the design variables. Numerical examples for shape optimizations of various inhomogeneities are presented to show the effectiveness of the present method.

2. Basic formulations

A set of $N$ inhomogeneities are embedded in an infinite heat conduction isotropic medium subjected to the remote heat flux as shown in Fig. 1. Each inhomogeneity with heat conductivity $k_i (i = 1, 2, \ldots, N)$ is assumed to be perfectly contacted with the isotropic matrix with the thermal conductivity $k_M$. An integral equation for the source point $P$ on the matrix side of
\[ \Gamma_j(j = 1, 2, \ldots, N) \] are the temperature and heat fluxes over the matrix interface under the far field. \( cM \) is the geometric-dependent constant at the source point \( P \) being on the inclusion–matrix interface \( \Gamma_j \). \( u_P(P) \) is the temperature on the source point \( P \) for all the bodies composed of the matrix material under the far field heat fluxes \( q^I_j \) and \( q^M_j \) for 2D or \( q^I_j, q^M_j \) and \( q^3_j \) for 3D. \( u_P(P) \) is the temperature and heat flux over the field point \( Q \) along \( \Gamma_j(j = 1, 2, \ldots, N) \). The fundamental solutions \( U_M \) and \( T_M \) for steady state systems are of the form \([14]\):

\[ U_M = \frac{1}{4\pi r} \quad \text{or} \quad T_M = \frac{1}{4\pi r} \quad \text{for three dimensional case} \quad (2a) \]

and

\[ U_M = \frac{1}{2\pi r} \ln \frac{r}{r_0} \quad \text{or} \quad T_M = \frac{1}{2\pi r} \ln \frac{r}{r_0} \quad \text{for two dimensional case} \quad (2b) \]

where \( r \) is the distance between the source point \( P \) and the field point \( Q \), \( n \) is the outward unit normal on \( \Gamma_j \), \( \partial r/\partial n = r_j n_i \) in which \( i = 1, 2 \) (2D) or \( i = 1, 2, 3 \) (3D). The Einstein summation convention of repeated indices is used here.

For the source point \( P \) on the inclusion side of \( \Gamma_j \), the corresponding integral equation is of the form

\[ cI(P)u_I(P) = \int_{\Gamma_j} U_j(P, Q)u_I(Q)d\Gamma_j - \int_{\Gamma_j} T_j(P, Q)u_I(Q)d\Gamma_j \quad (3) \]

and

\[ 0 = \int_{\Gamma_j} U_j(P, Q)u_I(Q)d\Gamma_j - \int_{\Gamma_j} T_j(P, Q)u_I(Q)d\Gamma_j \quad \text{for} \quad j \neq l \quad (4) \]

where \( cI(P) \) is the geometric-dependent constant at the source point \( P \) being on the inclusion–matrix interface \( \Gamma_j \). \( u_I(Q) \) and \( t_I(Q) \) are the temperature and heat flux over the field point \( Q \) along \( \Gamma_j(j = 1, 2, \ldots, N) \). \( u_j(Q) \) and \( t_j(Q) \) are the temperature and heat flux over the field point \( Q \) along \( \Gamma_j(j = 1, 2, \ldots, N) \). The fundamental solutions \( U_I, U_j, T_I \) and \( T_j \) for each inclusion are of the form \([14]\):

\[ U_I = \frac{1}{4\pi r} \quad \text{or} \quad T_I = \frac{1}{4\pi r} \quad \text{for three dimensional case} \quad (5a) \]

and

\[ U_I = \frac{1}{2\pi r} \ln \frac{r}{r_0} \quad \text{or} \quad T_I = \frac{1}{2\pi r} \ln \frac{r}{r_0} \quad \text{for two dimensional case} \quad (5b) \]

Using the following relationships, and adding (1), (3) and (4),

\[ k_j u_I = k_M u_M \]
\[ T_I = -T_M \]
\[ u_I = u_M \]
\[ t_I = -t_M \]

we can obtain the boundary integral formulation for steady state heat conduction which only contains the temperature on each inhomogeneity–matrix interface \([13]\):

\[ \left( cM(P) - \frac{k_I}{k_M} cI(P) \right) u_P(P) = u_P(P) - \int_{\Gamma_j} \left( 1 - \frac{k_I}{k_M} \right) T_j(P, Q)u_I(Q)d\Gamma_j \quad (7) \]

where \( T \) is the fundamental solution \( T_M \) of the matrix material (see Eq. (2)).

In the boundary element implementation of Eq. (7), isoparametric quadratic elements are used to discretize each inhomogeneity–matrix interface, i.e. \([15,16]\):

\[ x_u = N_l x_u^e \quad (8) \]

\[ u_l = N_l u_j^e \quad (9) \]

where \( a = 1, 2 \) (2D) or \( a = 1, 2, 3 \) (3D), and \( J = 1, 2, 3 \) (2D) or \( J = 1, \ldots, 8 \) (3D). \( N_j \) is the shape function for element node \( j \). \( x_u^e \) is a coordinate at node \( j \) in the element \( e \). \( u_l \) is a temperature at node \( j \) in the element \( e \). The discretization form of Eq. (7) for the source point \( P \) is obtained for 2D problems as follows:

\[ \left( cM(P) + \frac{k_I}{k_M} cI(P) \right) u^e(P) = u^e(P) - \sum_{j=1}^{N} \left( 1 - \frac{k_I}{k_M} \right) \int_{\Gamma_j} T_j(P, Q)u_I^e(Q)d\Gamma_j \quad (10a) \]

where \( |G| = x_u^e x_u^e = N_{il} N_{lj} x_u^e x_u^e \) in which \( x \) is a parameter coordinate in 2D space.

Similarly, the discretization equation for 3D problems is as follows:

\[ \left( cM(P) + \frac{k_I}{k_M} cI(P) \right) u^e(P) = u^e(P) - \sum_{j=1}^{N} \left( 1 - \frac{k_I}{k_M} \right) \int_{\Gamma_j} T_j(P, Q)u_I^e(Q)d\Gamma_j \quad (10b) \]

where \( |G|^2 = e_{ijkl} x_u^e x_u^e x_u^e x_u^e \) in which \( e \) is the permutation tensor, the subscripts \( i, j, k, l, m = 1, 2, 3 \), and \( i, j, K, L = 1, \ldots, 8 \).

Eq. (10) yields the system of boundary integral equations in the matrix form as

\[ AU = U^0 \quad (11) \]
where \( A \) is final coefficient matrix, \( U \) is a vector of temperatures, and \( U^0 \) is a known vector of temperatures in the matrix produced by the remote heat flux. Eq. (11) can then be solved for the unknown values of temperatures by standard matrix solution method. Note that the right hand side of Eq. (10) contains the singularity of \( O(1/r) \) for 2D or \( O(1/r^2) \) for 3D when the source point \( P \) approaches the field point \( Q \). These singular integrals can be indirectly calculated by the well-known method similar to the rigid body displacement method in elasticity [14].

The differential approach for shape optimizations of inhomogeneities needs the differentiation of Eq. (10) with respect to each design variable. In the present study, the design variable for 2D problems is chosen as the radial distance of each node from the center of its corresponding inhomogeneity. For 3D problems, only three semi-major axes of each ellipsoidal inhomogeneity are considered as the design variables. As a result, the discretized boundary integral sensitivity equation is as follows:

\[
\left( c_{st}(P) + \frac{k_s}{k_M} \xi(P) \right) u(P) + \left( \xi_{st}(P) + \frac{k_s}{k_M} \xi(P) \right) u(P) = U^0(P)
\]

\[
- \sum_{j=1}^{N} \left( 1 - \frac{k_j}{k_{M}} \right) s \int_{-1}^{1} T(P, Q) N_j \hat{u}^j d\xi
\]

\[
- \sum_{j=1}^{N} \left( 1 - \frac{k_j}{k_{M}} \right) s \int_{-1}^{1} \left( \hat{T}(P, Q) \hat{G} + T(P, Q) \hat{G} \right) N_j \hat{u}^j d\xi
\]

where the dot over some symbols denotes the derivative of related values with respect to the design variable. The derivatives of fundamental solution and other values with respect to design variable are given as follows:

\[
\hat{T} = \frac{1}{2\pi r} \left( \frac{\partial r}{\partial n} \right) \tag{13a}
\]

\[
\hat{T} = \frac{1}{4\pi r^2} \left( \frac{\partial r}{\partial n} \right) \tag{13b}
\]

\[
|\hat{G}| = \left| \frac{1}{|G|} N_i \xi_j x_{ij} \right| \tag{14a}
\]

\[
|\hat{G}| = \varepsilon_{ijk} n_i (x_{jx} + x_{kx}) \tag{14b}
\]
where $\mathbf{U}^0$ is the derivative of $\mathbf{U}$ with respect to design variables, respectively.

If the coefficient matrix $\mathbf{A}$ of Eq. (11) is decomposed into $\mathbf{LU}$, then during solving Eq. (16) only the terms of $\mathbf{AU}$ and $\mathbf{U}^0$ need to be formed. It is also mentioned here that the coefficient matrix $\mathbf{A}$ in Eq. (16) includes singularity of $O(1/r)$ for 2D or $O(1/r^3)$ for 3D when the source point $P$ approaches the field point $Q$. The corresponding solution technique is the same as that of singular integral appearing in Eq. (10).

For steady state heat conduction inhomogeneous medium, the shape optimization of inhomogeneities may be expressed as

$$\text{Min } E(\mathbf{b})$$

Subjected to:

$$h_1(\mathbf{b}) = C_i, i = 1, 2, \ldots, N$$

$$b_k^{\text{min}} \leq b_k \leq b_k^{\text{max}}, k = 1, 2, n$$

where $C_i$ is the given area (2D)/volume (3D) of the $i$th inhomogeneity in all the inhomogeneities with $N$ being the number of inhomogeneities. $\mathbf{b}$ is the design variable vector with $n$ being the number of design variables, and $b_k^{\text{min}}$ and $b_k^{\text{max}}$ are the lower and the upper limits of design variable $b_k$. The objective function $E$ is the heat energy increment of the composite system due to the existence of inhomogeneities, i.e. [17]

$$\Delta W = \frac{1}{2} \sum_{j=1}^{N} \int_{\Gamma_j} (n_i q_i^0 u - n_i q_i^0 u) d\Gamma$$

Eq. (12) can be written in a matrix form as

$$\mathbf{AU} + \Delta \mathbf{U} = \mathbf{U}^0$$

or

$$\mathbf{AU} = \mathbf{U}^0 - \Delta \mathbf{U}$$

where $\mathbf{A}$, $\mathbf{U}$ and $\mathbf{U}^0$ are the derivatives of $\mathbf{A}$, $\mathbf{U}$ and $\mathbf{U}^0$ with respect to design variables, respectively.

$\mathbf{U}^0 = -\frac{1}{k_0} \mathbf{q}_0 \mathbf{x}_0$

Fig. 3. Variation of heat energy increment with iterative number for each case: (1) $k_i/k_M = 0.0$, $q_i^0 = 1$ and $q_i^0 = 0$; (2) $k_i/k_M = 10.0$, $q_i^0 = 1$ and $q_i^0 = 0$; (3) $k_i/k_M = 0.0$, $q_i^0 = 1$ and $q_i^0 = 1$; and (4) $k_i/k_M = 10.0$, $q_i^0 = 1$ and $q_i^0 = 1$.

Fig. 4. Optimal processes of inhomogeneity with different heat conductivities for different heat fluxes: (a) $k_i/k_M = 0.0$, $q_i^0 = 1$, $q_i^0 = 0$; (b) $k_i/k_M = 10.0$, $q_i^0 = 1$, $q_i^0 = 0$; (c) $k_i/k_M = 0.0$, $q_i^0 = q_i^0 = 1$; and (d) $k_i/k_M = 10.0$, $q_i^0 = q_i^0 = 1$. 

Subjected to:

$$h_1(\mathbf{b}) = C_i, i = 1, 2, \ldots, N$$

$$b_k^{\text{min}} \leq b_k \leq b_k^{\text{max}}, k = 1, 2, n$$

where $C_i$ is the given area (2D)/volume (3D) of the $i$th inhomogeneity in all the inhomogeneities with $N$ being the number of inhomogeneities. $\mathbf{b}$ is the design variable vector with $n$ being the number of design variables, and $b_k^{\text{min}}$ and $b_k^{\text{max}}$ are the lower and the upper limits of design variable $b_k$. The objective function $E$ is the heat energy increment of the composite system due to the existence of inhomogeneities, i.e. [17]

$$\Delta W = \frac{1}{2} \sum_{j=1}^{N} \int_{\Gamma_j} (n_i q_i^0 u - n_i q_i^0 u) d\Gamma$$

or

$$\mathbf{AU} = \mathbf{U}^0 - \Delta \mathbf{U}$$

where $\mathbf{A}$, $\mathbf{U}$ and $\mathbf{U}^0$ are the derivatives of $\mathbf{A}$, $\mathbf{U}$ and $\mathbf{U}^0$ with respect to design variables, respectively.
where \( u^0 \) is the uniform temperature field, \( q^0 \) is a constant heat flux. \( n_i \) is the component of a unit outer normal vector to the surface of the \( j \)-th inclusion. \( u \) is the actual temperature on the interface \( \Gamma_j \). \( t_i(i=x,y,z) \) is the heat flux component on the interface \( \Gamma_j \).

The second integral term in (18) can be written as

\[
\int_{\Gamma_J} n_i u_i^0 d\Gamma = \int_{\Omega} t_i u_i^0 dV = -\int_{\Omega} k_i u_i u_i^0 dV \\
= -\frac{k_i}{k_{M,j}} \int_{\Omega} k_M u_i u_i^0 dV = \frac{k_i}{k_{M,j}} \int_{\Omega} q_i^0 u_i^0 dV \\
= \frac{k_i}{k_{M,j}} \int_{\Omega} q_i^0 u_i^0 dV \\
= \frac{k_i}{k_{M,j}} \int_{\Gamma} n_i q_i^0 u_i d\Gamma \\
\]

where the heat equilibrium relationships, i.e. \( t_i = 0 \) and \( q_i^0 = 0 \), have been used.

Therefore, we can obtain the following equation from Eq. (18):

\[
E = \frac{1}{2K_M} \sum_{j=1}^{N} \left\{ (k_M - k_j) \int_{\Gamma_j} n_i q_i^0 u_i d\Gamma \right\} 
\]

Fig. 5. Comparisons of shape optimizations of inhomogeneity from MMA and NCONF: (a) \( k_i/k_M = 0.0, q_i^0 = 1, q^0 = 0 \); (b) \( k_i/k_M = 10.0, q_i^0 = 1, q^0 = 0 \); (c) \( k_i/k_M = 0.0, q_i^0 = q^0 = 1 \); and (d) \( k_i/k_M = 10.0, q_i^0 = q^0 = 1 \).

Fig. 6. Variation of heat energy increment with iterative number for two cases: (1) \( k_i/k_M = 2.0 \) and (2) \( k_i/k_M = 10.0 \).
Fig. 7. Optimal processes of inhomogeneity for $q_0^x = x$ and $q_0^y = 0.5$ based on the MMA: (a) $k_I/k_M = 2.0$ and (b) $k_I/k_M = 10.0$.

Fig. 8. Optimal processes of inhomogeneity for $q_0^x = x$ and $q_0^y = 0.5$ based on the NCONF: (a) $k_I/k_M = 2.0$; and (b) $k_I/k_M = 10.0$.

Fig. 9. Comparisons of optimal shapes of inhomogeneity for $q_0^x = x$ and $q_0^y = 0.5$ from the MMA and the NCONF: (a) $k_I/k_M = 2.0$ and (b) $k_I/k_M = 10.0$. 
The ith constrained function is expressed as

\[ h_i = \int_{V_i} dV = \frac{1}{3} \int_{S_i} x_i n_i dS \]  \hspace{1cm} \text{for 3D} \tag{21a} \]

or

\[ h_i = \int_{S_i} dS = \frac{1}{2} \int_{S_i} x_1 n_1 dS \]  \hspace{1cm} \text{for 2D} \tag{21b} \]

where the subscripts \( V_i \) and \( S_i \) are respectively the volume (3D) and the area (2D) of the ith inhomogeneity.

Various optimization techniques can be used to solve the above optimization problems, e.g., genetic algorithms [18] and sequential quadratic programming [19]. In this paper, the MMA proposed by Svanberg [20] is used. We use the change of the objective function values as the convergence criteria, i.e.

\[ \frac{E^{(k)} - E^{(k-1)}}{E^{(k)}} \leq \epsilon \] \hspace{1cm} \text{(22)}

where the superscript \( k \) denotes the objective functional value at the \( k \)th iteration, \( \epsilon \) is a given small number, i.e. \( \epsilon = 10^{-4} \).

In the MMA, the derivatives of the objective function and the constrained functions with respect to design variables are needed, i.e.

\[ \dot{E} = \frac{1}{2 k_{\mu}} \sum_{i=1}^{N} \left( (k_{\mu} - k_i) \sum_{j=1}^{N} \int_{dV} \left( \dot{\hat{n}} q_i^{(\mu)} G_i + n_i q_i^{(\mu)} G_i \right) u + n_i q_i^{(\mu)} G_i \dot{u} \right) dV \] \hspace{1cm} \text{(23)}

and

\[ h_i = \frac{1}{2} \int_{S_i} \left[ (\dot{x}_n n_n + x_n \hat{n}_n) G_i + x_n n_n G_i \right] dS \] \hspace{1cm} \text{for 2D} \tag{24a} \]

\[ h_i = \frac{1}{2} \int_{S_i} \left[ (\dot{x}_n n_n + x_n \hat{n}_n) G_i + x_n n_n G_i \right] dS \] \hspace{1cm} \text{for 2D} \tag{24b} \]

where \( n_1 = n_2 / G_i (n_1 \dot{x}_1 + n_2 \dot{x}_2) \text{ and } n_2 = - (n_1 / G_i (n_1 \dot{x}_1 + n_2 \dot{x}_2)) \) for 2D medium. For 3D problem, we have \( n_1 = n_2 / G_i (\epsilon_{ijk} (\dot{x}_j \dot{x}_k + \dot{x}_j \dot{x}_k) - \dot{n}_i n_j \dot{n}_k \dot{x}_j \dot{x}_k / G_i (n_1 \dot{x}_1 + n_2 \dot{x}_2) n_1 \dot{x}_1 + n_2 \dot{x}_2) \).

3. Numerical examples

To show the effectiveness of the BEM and the optimization technique presented in this paper, some numerical examples are used to show the shape optimizations of various inhomogeneities embedded in an infinite isotropic steady state heat conduction media subjected to remote heat flux. Quadratic isoparametric boundary elements with 3 (2D) or 8 (3D) nodes are adopted to discretize each inhomogeneity–matrix interface. The matrix and the inhomogeneities are assumed to be isotropic. The heat conductivity of the matrix is taken as \( k_{\mu} = 1 \), and the heat conductivities of the inhomogeneities

Fig. 10. Optimal shapes of inhomogeneity with different heat conductivities for different heat fluxes: (a) \( k_i / k_{\mu} = 0.0, q_i^0 = 1, q_i^0 = 0 \); (b) \( k_i / k_{\mu} = 10.0, q_i^0 = 1, q_i^0 = 0 \); (c) \( k_i / k_{\mu} = 0.0, q_i^0 = d_i^0 = 1 \); and (d) \( k_i / k_{\mu} = 10.0, q_i^0 = d_i^0 = 1 \).
can be taken as various values, i.e. \( k_I / k_M = 0.0, 0.5, 2.0 \) and 10. Each constrained area (2D) or volume (3D) is assumed as 6.28 unless otherwise stated. Design variables are taken as \( r_{bk} r_1 \) for 2D and \( \min(a, b, c) \leq b_k \leq \max(a, b, c) \) (\( k = 1, 2, \ldots, n \), in which \( n \) is node number) for 3D. All units are assumed to be consistent and all variables are considered as dimensionless ones.

Fig. 11. Optimal shapes of inhomogeneities with different heat conductivities for different constrained areas and different heat fluxes: (a) \( k_I / k_M = 0.0, q_0^x = 1, q_0^y = 0 \); (b) \( k_I / k_M = 10.0, q_0^x = 1, q_0^y = 0 \); (c) \( k_I / k_M = 0.0, q_0^x = q_0^y = 1 \); (d) and \( k_I / k_M = 10.0, q_0^x = q_0^y = 1 \).

Fig. 12. Variations of the heat energy increment with iterative number for two inhomogeneities: (a) \( q_0^x = 1, q_0^y = 0 \) and (b) \( q_0^x = q_0^y = 1 \).
Fig. 13. Optimal shapes of two inhomogeneities with different heat conductivities for different remote heat fluxes, i.e. (a) \( q_{0x} = 1 \), \( q_{0y} = 0 \) and (b) \( q_{0x} = 1 \), \( q_{0y} = 1 \).

Fig. 14. Variations of the heat energy increment with iterative number for the left cavity and the right inhomogeneity: (a) \( q_{0x} = 1 \), \( q_{0y} = 0 \) and (b) \( q_{0x} = q_{0y} = 1 \).

Fig. 15. Optimal shapes of one cavity (left) and one inhomogeneity (right) with different heat conductivities for different heat fluxes, i.e. (a) \( q_{0x} = 1 \), \( q_{0y} = 0 \) and (b) \( q_{0x} = q_{0y} = 1 \).
expresses and the successive quadratic programming algorithm with a subdomain boundary element method, i.e. SBEM (see Appendix), optimizations of single inhomogeneity with different heat conductivities taken as 1.

inhomogeneity. Fig. 3 shows the variation of heat energy increment with iterative number for four inhomogeneities: (a) \( q_1^0 = 1 \), \( q_2^0 = 0 \) and (b) \( q_1^0 = q_2^0 = 1 \).

3.1. Shape optimization of single 2D inhomogeneity

One 2D inhomogeneity is embedded in an infinite isotropic steady state heat conduction medium subjected to remote heat flux, i.e. \( q_i^0 = q_j^0 = 1 \) or \( q_i^0 = 1, q_j^0 = 0 \). All the design variables are initially taken as 1.

To illustrate the rightness of the present method, the shape optimizations of single inhomogeneity with different heat conductivities under various remote heat fluxes are also shown in Fig. 2 using the subdomain boundary element method, i.e. SBEM (see Appendix), and the successive quadratic programming algorithm with a finite difference gradient (the corresponding optimal code NCONF is available [21]). In the calculation, 64 nodes are chosen to carry out the shape optimizations of this inhomogeneity. One can observe that the results from these two methods are in excellent agreement.

In order to check the convergence property of the MMA, 64 nodes are also chosen to carry out the shape optimization of this inhomogeneity. Fig. 3 shows the variation of heat energy increment with iterative number for each case, i.e. case 1 represents \( k_i/k_M = 0.0, q_1^0 = 1 \) and \( q_2^0 = 0 \); case 2 is for \( k_i/k_M = 10.0, q_1^0 = 1 \) and \( q_2^0 = 0 \); case 3 denotes \( k_i/k_M = 0.0, q_1^0 = 1 \) and \( q_2^0 = 1 \); case 4 expresses \( k_i/k_M = 10.0, q_1^0 = 1 \) and \( q_2^0 = 1 \).

One can observe that two optimal methods result in almost the same optimal shape from different heat conductivities and heat fluxes, i.e. (a) \( q_1^0 = 1, q_2^0 = 0 \) and (b) \( q_1^0 = 1, q_2^0 = 1 \).

Fig. 4(a) shows that when the iterative number is equal to 8, the optimal shape of inhomogeneity can be attained when the iterative number is 21. Fig. 4(b) displays that for \( k_i/k_M = 10.0, q_2^0 = 1 \) and \( q_2^0 = 0 \), the optimal shape of inhomogeneity can be attained when the iterative number is 21. Fig. 4(c) and (d) illustrates the optimal shape of inhomogeneity for two other cases, i.e. (1) \( k_i/k_M = 0.0, q_2^0 = q_3^0 = 1 \) (iterative number 8) and (2) \( k_i/k_M = 0.0, q_2^0 = q_3^0 = 1 \) (iterative number 21).

Fig. 5 shows some comparisons for the shape optimizations of inhomogeneity from the MMA and the successive quadratic programming algorithm with a finite difference gradient (the corresponding optimal code NCONF is available [21]). One can observe that two optimal methods result in almost the same optimal shape from different heat conductivities and heat fluxes, though the iterative numbers for convergence solutions are different.

For heat fluxes \( q_1^0 = x \) (\( x \) is a dimensionless variable) and \( q_2^0 = 0.5 \) as well as the constrained area is assumed to be 3.14, the variation of the heat energy increment with iterative number in the MMA is displayed in Fig. 6. One can observe that the convergence solution can be obtained for \( k_i/k_M = 2.0 \) and \( k_i/k_M = 10.0 \) when the iterative numbers are 8 and 21.
respectively. The shape optimization processes are shown in Fig. 7 (MMA) and Fig. 8 (NCONF). We can find that the optimal shape from the MMA can be obtained when the iterative number arrives at 11 for $k_I/k_M = 2$: $0$ or 22 for $k_I/k_M = 10$: $0$. Whereas the optimal shape from the NCONF can be attained when the iterative number is 28 for $k_I/k_M = 2$: $0$ or 18 for $k_I/k_M = 10$: $0$. As a comparison, the optimal shapes from the MMA and the NCONF are given in Fig. 9. One can see that the resulting optimal shapes are almost the same for two optimal methods, though the iterative numbers are different.

In order to check the effect of design variable number on the shape optimization of inhomogeneity, 32 and 64 nodes (radial distance at each node is considered as design variable) are adopted which result in almost the same optimal shape for different heat fluxes (see Fig. 10). In the following 2D examples containing more inhomogeneities, we adopt 32 nodes, i.e. 32 design variables, to carry out the simulation of the shape optimizations of various inhomogeneities. For the inhomogeneity with $k_I/k_M = 0.0$, i.e. hole, the optimal shape becomes slender in the direction of the resultant of heat fluxes $q_0^x$ and $q_0^y$ (see Fig. 10(a) and (c)). On the contrary, if the inhomogeneity with $k_I/k_M = 10.0$ is adopted, the optimal shape becomes slender in the vertical direction of the resultant of heat fluxes $q_0^z$ and $q_0^y$ (see Fig. 10(b) and (d)). These results are similar to those for elastic inclusion optimal shapes [22]. Fig. 11 demonstrates the optimal shapes of inhomogeneity with different heat conductivities for different constrained areas and different heat fluxes. Two different constrained areas result in the same optimal shape.

3.2. Optimal shapes of two inhomogeneities

Two inhomogeneities are embedded in an infinite isotropic steady state medium subjected to remote heat flux $q_0^z = q_0^y = 1$ or 0.
q_y^0 = 1, q_z^0 = 0. The distance between the centers of two inhomogeneities is taken as 5. Following the above example, 32 nodes, i.e. 32 design variables, of each inhomogeneity are used to carry out the boundary element analysis and all design variables are initially taken as 1.

The variations of the heat energy increment with iterative number are shown in Fig. 12(a) and (b), respectively, for inhomogeneities with different heat conductivities under q_x^0 = 1, q_y^0 = 0 and q_z^0 = q_y^0 = 1. One can observe from Fig. 13(a) that the optimal shapes of two inhomogeneities become slender along q_x^0 direction for K_I/ K_M < 1.0 and q_y^0 = 1, q_z^0 = 0, whereas for K_I/ K_M > 1.0 and q_y^0 = 1, q_z^0 = 0, the optimal shapes of two inhomogeneities become slender along the direction being vertical to q_y^0. Fig. 13(b) displays the optimal shapes of two inhomogeneities for q_x^0 = q_y^0 = 1. Different from the case, i.e. q_x^0 = 1, q_y^0 = 0, the slender direction of the optimal shapes of two inhomogeneities is not again directing to q_y^0, whereas it has a rotation angle with q_y^0 depending on heat conductivities.

Fig. 14(a) and (b) displays variations of the heat energy increment with iterative number for the left cavity and the right inhomogeneities under q_x^0 = 1, q_y^0 = 0 and q_z^0 = q_y^0 = 1. Fig. 15(a) illustrates that the optimal shapes of cavity and inhomogeneities, respectively, with various heat conductivities subjected to heat flux q_x^0 = 1, q_y^0 = 0, whereas Fig. 15(b) shows those for q_x^0 = q_y^0 = 1. In all the calculations for the same heat flux, one can find that under each case, i.e. K_I/ K_M < 1.0 or K_I/ K_M > 1.0, the heat conductivities within two cases (e.g. K_I/ K_M = 0.0, 0.5 < 1.0 or K_I/ K_M = 2.0, 10.0 > 1.0) have less influence on the final optimal shapes of inhomogeneities.

### 3.3. Optimal shapes of four inhomogeneities

The center coordinates of four inhomogeneities embedded in an infinite isotropic matrix are at (−2.5, 2.5), (2.5, 2.5), (2.5, −2.5) and (−2.5, −2.5), respectively. Two heat fluxes, i.e. q_x^0 = 1, q_y^0 = 0 and q_x^0 = q_y^0 = 1 are considered. Similar to the above two examples, 32 nodes, i.e. 32 design variables, of each inhomogeneity are used and all the design variables are initially considered as 1. Fig. 16(a) and (b) shows the variations of the heat energy increments with iterative number for four inhomogeneities under heat fluxes q_x^0 = 1, q_y^0 = 0 and q_x^0 = q_y^0 = 1. Optimal shapes of four inhomogeneities are shown in Fig. 17(a) and (b), respectively. One can see that for q_x^0 = 1, q_y^0 = 0, the optimal shape of each inhomogeneity becomes slender along the direction q_x^0 for K_I/ K_M < 1.0, whereas the optimal shape of each inhomogeneity becomes slender along the direction being vertical to q_x^0 for K_I/ K_M > 1.0. For q_x^0 = q_y^0 = 1, the optimal shape of each inhomogeneity becomes slender along the direction being vertical to q_x^0 for K_I/ K_M < 1.0, whereas the optimal shape of each inhomogeneity becomes slender along the direction q_x^0 for K_I/ K_M > 1.0. For q_x^0 = q_y^0 = 1, the optimal shape of each inhomogeneity becomes slender along the direction being vertical to q_x^0 for K_I/ K_M < 1.0, whereas the optimal shape of each inhomogeneity becomes slender along the direction q_x^0 for K_I/ K_M > 1.0.

---

**Fig. 20.** Two ellipsoids: (a) original ellipsoids; (b) optimal shapes for q_x^0 = q_y^0 = 1 and K_I/ K_M = 0.0 as well as K_I/ K_M = 10.0; (c) optimal shapes for q_x^0 = q_y^0 = 0, q_z^0 = 1 and K_I/ K_M = 10.0; and (d) optimal shapes for q_x^0 = q_y^0 = 0, q_z^0 = q_y^0 = 1 and K_I/ K_M = 10.0.

**Fig. 21.** Variation of the heat energy increment with iterative number for two ellipsoids: (1) q_x^0 = q_y^0 = q_z^0 = 1 and K_I/ K_M = 0.0; (2) q_x^0 = q_y^0 = q_z^0 = 1 and K_I/ K_M = 10.0; (3) q_x^0 = 0, q_y^0 = 0, q_z^0 = 1 and K_I/ K_M = 0.0; and (4) q_x^0 = 0, q_y^0 = 0, q_z^0 = 1 and K_I/ K_M = 10.0.
omogeneity becomes slender along an angle (＜90° for \( K_I/K_M < 1.0 \) or ＞90° for \( K_I/K_M > 1.0 \) ) with respect to the \( q_0^i \) direction.

3.4. Optimal shape of single ellipsoid

One ellipsoid is embedded in an infinite isotropic medium subjected to different heat fluxes, i.e. \( q_0^i = 0, q_0^j = 0, q_0^k = 1 \) or \( q_0^i = q_0^j = q_0^k = 1 \). Three semi-major axes along the axes \( x, y \) and \( z \) are assumed to be 1.8, 2.0 and 1.2, respectively. In the calculation, 96 quadratic isoparametric quadrilateral elements with 290 nodes are adopted for the ellipsoid (see Fig. 18(a)). When \( q_0^i = q_0^j = q_0^k = 1 \) and the heat energy increment approaches the minimum, the ellipsoidal cavity becomes one approximate spherical cavity with three semi-major axes along the axes \( x, y \) and \( z \), i.e. 1.627, 1.663 and 1.600 (see Fig. 18(b)). Similarly, the ellipsoid with heat conductivity \( K_I/K_M = 10.0 \) also becomes one approximate sphere with three semi-major axes along the axes \( x, y \) and \( z \), i.e. 1.632, 1.640 and 1.617. When \( q_0^i = 0, q_0^j = 0, q_0^k = 1 \) and the heat energy increment approaches the minimum, the ellipsoidal cavity is still one ellipsoidal cavity, but its maximum semi-major axis is transferred to the \( z \) direction, i.e. heat flux direction \( q_0^i \). Its three semi-major axes along the axes \( x, y \) and \( z \) are respectively 1.348, 1.607 and 2.0 (see Fig. 18(c)). However, the ellipsoid with heat conductivity \( K_I/K_M = 10.0 \) is also one ellipsoid with three semi-major axes along the axes \( x, y \) and \( z \), i.e. 1.818, 1.996 and 1.20 (see Fig. 18(d)). We also calculate two ellipsoidal cases, i.e. \( K_I/K_M = 0.2 \) and \( K_I/K_M = 2.0 \), for \( q_0^i = 0, q_0^j = 0, q_0^k = 1 \). The final optimal results are still ellipsoids with three semi-major axes along the axes \( x, y \) and \( z \), i.e. 1.348, 1.607 and 2.0 (\( K_I/K_M = 0.2 \)) as well as 1.815, 1.999 and 1.20 (\( K_I/K_M = 0.2 \)). Fig. 19 shows the variation of the heat energy increment with iterative number for four cases, i.e. (1) \( q_0^i = q_0^j = q_0^k = 1 \) and \( K_I/K_M = 0.0 \); (2) \( q_0^i = q_0^j = q_0^k = 1 \) and \( K_I/K_M = 10.0 \); (3) \( q_0^i = 0, q_0^j = 0, q_0^k = 1 \) and \( K_I/K_M = 0.0 \); (4) \( q_0^i = 0, q_0^j = 0, q_0^k = 1 \) and \( K_I/K_M = 10.0 \).

3.5. Optimal shape of two ellipsoids

Fig. 20(a) displays that two ellipsoids are embedded into an infinite isotropic medium subjected to different heat fluxes, i.e. \( q_0^i = 0, q_0^j = 0, q_0^k = 1 \) or \( q_0^i = q_0^j = q_0^k = 1 \). Each ellipsoid has the same geometrical size as the above example. The distance between centers of two ellipsoids is taken as 4.5 along the axis \( x \). For \( q_0^i = q_0^j = q_0^k = 1 \), when the minimum heat energy is approached, two new ellipsoids are obtained with three semi-major axes along the axes \( x, y \) and \( z \), i.e. 1.513, 1.725 and 1.658 (\( K_I/K_M = 0.0 \)) as well as 1.509, 1.701 and 1.686 (\( K_I/K_M = 10.0 \)) as shown in Fig. 20(b). When \( q_0^i = 0, q_0^j = 0, q_0^k = 1 \), we obtain two optimal ellipsoidal shapes with three semi-major axes along the axes \( x, y \) and \( z \), i.e. 1.292, 1.676 and 2.0 (\( K_I/K_M = 0.0 \)) as well as 2.0, 1.814 and 1.2 (\( K_I/K_M = 10.0 \)). Fig. 21 presents the variation of the heat energy increment with iterative number for two ellipsoids in four cases, i.e. (1) \( q_0^i = q_0^j = q_0^k = 1 \) and \( K_I/K_M = 0.0 \); (2) \( q_0^i = q_0^j = q_0^k = 1 \) and \( K_I/K_M = 10.0 \); (3) \( q_0^i = 0, q_0^j = 0, q_0^k = 1 \) and \( K_I/K_M = 0.0 \); and (4) \( q_0^i = 0, q_0^j = 0, q_0^k = 1 \) and \( K_I/K_M = 10.0 \).

4. Conclusions

The shape optimizations of various inhomogeneities embedded in the infinite isotropic medium subjected to remote heat flux have been investigated by the BEM and the MMA. The boundary integral equations and the heat energy increment formulations used in this paper only contain the temperature on each matrix—inhomogeneity interface. These formulations are especially suitable for the shape optimization analysis of steady state heat conduction inhomogeneous problems. Examples are presented to show the shape optimizations of various inhomogeneities in 2D and 3D problems.

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Appendix. Shape optimizations for steady state heat conductivity using subdomain boundary element method

Referring to Eq. (1), we can obtain a set of linear equations in the form (for simplicity, the derivation of the related equations is given for single inclusion embedded in an infinite domain.}

\[
H_M u_M = G_M t_M + u_M^0
\]

(25)

where \( u_M^0 \) is a known vector of temperatures in the matrix produced by the remote heat flux. The square matrix \( H_M \) contains all integrals of the \( T \) kernel plus the jump term \( C_M \). The matrix \( G_M \) involves all the integrals of the \( U \) kernel. \( u_M \) and \( t_M \) are nodal temperature and heat flux on the matrix side of the interface \( \Gamma \), respectively.

Referring to Eq. (3), we can attain the following system of equations for the inclusion:

\[
H_I u_I = G_I t_I
\]

(26)

where the square matrix \( H_I \) contains all integrals of the \( T \) kernel plus the jump term \( C_I \). The matrix \( G_I \) involves all the integrals of the \( U \) kernel. \( u_I \) and \( t_I \) are nodal temperature and heat flux on the inclusion side of the interface \( \Gamma \), respectively.

The inclusion–matrix interface \( \Gamma \) is assumed to be ideal contact. Thus, we have the following relationships:

\[
u_I = u_M \]
\[
t_I = -t_M
\]

(27)

From Eq. (26), one can obtain

\[
u_I = H_I^{-1} G_I t_I = -H_I^{-1} G_I t_M
\]

(28)

Substituting Eq. (28) into Eq. (26) one obtains

\[
(G_M + H_M H_I^{-1} G_I) t_M = -u_M^0
\]

(29)

Solving the above system all the interface values \( t_M \), i.e. \( -t_M \), are fully determined. Then substituting \( K_M \) into Eq. (28) all the interface values \( u_I \), i.e. \( u_M \), can be obtained. One can now substitute \( u_I \) and \( t_I \) into Eq. (18) to obtain the heat energy increment of the composite system. Based on optimization methods, i.e. the successive quadratic programming algorithm with a finite difference gradient [21], the shape optimizations of inhomogeneities for steady state heat conduction in an infinite medium can be done.

References