First- and second-order sensitivity analysis schemes by collocation-type Trefftz method

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This paper presents the boundary-type schemes of the first- and the second-order sensitivity analyses by Trefftz method. In the Trefftz method, physical quantities are approximated by the superposition of the T-complete functions satisfying the governing equations. Since the T-complete functions are regular, the approximate expressions of the quantities are also regular. Therefore, direct differentiation of them leads to the expressions of the sensitivities.

Firstly, the Trefftz method for the two-dimensional potential problem is formulated by means of the collocation method. Then, the first- and the second-order sensitivity analysis schemes are explained with the simple numerical examples for their verification.

1. INTRODUCTION

Shape optimization problems of the structures and the machine elements are often solved by applying the gradient-type search schemes. The search schemes generally employ the first-order derivatives of the object functions (sensitivities) and therefore, many researchers have been studying the first-order sensitivity analysis schemes based on finite element, boundary element and Trefftz methods[1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14]. By the way, some researchers have presented the search schemes using, in addition to the first-order sensitivities, the second-order sensitivities and the second-order sensitivity analysis schemes based on the finite and boundary element methods[15, 16, 17, 18, 19, 20, 21, 22, 23, 24]. The search schemes using both first- and second-order sensitivities, as mentioned by Mlejnek[23], have faster and stabler convergency property than the ordinary schemes using the first-order sensitivities alone. However, the formulation of the second-order sensitivity analysis is very complicated and moreover, its computational cost is relatively high. For overcoming the difficulties, this paper presents the second-order sensitivity analysis schemes by the Trefftz method.

The Trefftz method is formulated by introducing the regular T-complete functions satisfying the governing equations. Physical quantities are approximated by the superposition of the T-complete functions. Since the T-complete functions are regular, the approximate expressions are also regular. Direct differentiation of the quantities leads to the regular expressions of the first- and second-order sensitivities.

This paper is organized as follows. Firstly, the present scheme is compared with the other schemes based on the finite and the boundary element methods. The Trefftz method for the two-dimensional potential problem is formulated by means of the collocation method. Then, the first-
and the second-order sensitivity analysis schemes are explained. Finally, the schemes are applied to the simple numerical examples in order to confirm the validity.

2. Sensitivity Analysis Schemes

In this section, we shall compare the present scheme with the ordinary schemes based on the finite and the boundary element methods (Table 1).

<table>
<thead>
<tr>
<th>Solver type</th>
<th>Accuracy</th>
<th>Formulation</th>
</tr>
</thead>
<tbody>
<tr>
<td>FEM</td>
<td>Domain-type</td>
<td>Lower</td>
</tr>
<tr>
<td>BEM</td>
<td>Boundary-type</td>
<td>Complicated</td>
</tr>
<tr>
<td>Trefftz method</td>
<td>Boundary-type</td>
<td>Simple</td>
</tr>
</tbody>
</table>

2.1. Finite element method

The finite element method is a very powerful tool for numerical analysis. Since, however, the domain under consideration is discretized by the finite elements, the input-data generation is very difficult. Besides, physical quantities are approximated by the linear combination of the interpolation functions with nodal values. Since the interpolation functions are generally low-order polynomials of the coordinates, the sensitivities, which are derived from the differentiation of the quantities, are approximated by the lower-order interpolation functions than that of the original quantities. Especially, in the second-order sensitivity analysis, the interpolation functions are differentiated twice and therefore, the relatively high-order interpolation functions have to be used for approximating the original quantities.

2.2. Boundary element method

Since the boundary element method is known as the boundary-type solution, the input-data generation is much simpler than the domain-type solutions such as the finite difference and the finite element methods. The singularity of the integral equations, however, is a great difficulty. Quantities are expressed by the singular integral equations. Therefore, the sensitivities are expressed by the hyper-singularity equations derived from the differentiation of the original equations. For the regularization of the hyper-singular equations, we have to apply special formulations[2, 5, 8, 9, 10, 11]. Such formulations, however, are very complicated.

2.3. Trefftz method

Since the Trefftz method is classified into the boundary-type solution, the input-data generation is easier than the domain-type solutions. Quantities are approximated by the superposition of the T-complete functions. The T-complete functions are not dependent on the shape parameters and therefore, the accuracy of the sensitivities is not reduced by the differentiation of the quantities. Since the T-complete functions are regular, the sensitivities are expressed by the regular expressions. Therefore, unlike the boundary element method, they can be estimated easily without special formulations.

3. Trefftz Formulation

3.1. Governing equation and T-complete function

The governing equation and the boundary condition of the two-dimensional potential problem are written as follows.
\[ \nabla^2 u = 0 \quad \text{(in } \Omega) \text{,} \]

\[ u = \bar{u} \quad \text{(on } \Gamma_1) \text{,} \]

\[ q = \frac{\partial u}{\partial \tilde{n}} = \bar{q} \quad \text{(on } \Gamma_2) \text{,} \]

where \( u \) and \( q \) are the potential and its normal derivative on the boundary (flux), respectively. \( \Omega, \Gamma_1 \) and \( \Gamma_2 \) denote the domain occupied by the object under consideration, its potential- and the flux-specified boundaries, respectively. \( \tilde{n} \) is the outward unit vector in the normal direction on the boundary and \( (\bar{\cdot}) \) the specified value on the boundary.

The Trefftz method is formulated by introducing the T-complete functions \( u^*_n \). \( u^*_n \) is a regular function satisfying the governing equation:

\[ \nabla^2 u^*_n = 0 \quad (n = 1, 2, \cdots) \text{.} \]

The T-complete functions for the two-dimensional potential problems in the bounded region are defined as \([25, 26, 27]\):

\[ u^* = \{u_1, u_2, u_3, \cdots, u_{2n}, u_{2n+1}, \cdots\}^T \]

\[ = \{1, r \Re e^{j\theta}, r^2 \Re e^{j\theta}, \cdots, r^n \Re e^{j\theta}, r^n \Im e^{j\theta}, \cdots\}^T \quad (n = 1, 2, \cdots) \text{,} \]

where \( j \) is the imaginary unit and then, \( r \) and \( \theta \) are the plane polar coordinates whose origin is taken arbitrarily.

### 3.2. Collocation formulation

The potential \( u \) is approximated by the superposition of the T-complete functions \( u^*_n \) with unknown parameters \( a_n \);

\[ u \simeq \bar{u} = a_1 u_1^* + a_2 u_2^* + \cdots + a_N u_N^* = a^T u^*. \]

By differentiating this equation with respect to the normal direction on the boundary, we have the approximate expression of the flux

\[ q \simeq \bar{q} \equiv \frac{\partial \bar{u}}{\partial \tilde{n}} = a_1 q_1^* + a_2 q_2^* + \cdots + a_N q_N^* = a^T q^*. \]

Since the above approximate solutions do not satisfy the boundary condition (2), the residuals yield:

\[ R_1 \equiv \bar{u} - \bar{u} = a^T u^* - \bar{u} \neq 0 \quad \text{on } \Gamma_1 \text{,} \]

\[ R_2 \equiv \bar{q} - \bar{q} = a^T q^* - \bar{q} \neq 0 \quad \text{on } \Gamma_2 \text{.} \]

In the collocation method, the residual on the collocation point \( P_m \) disappears. From Eq. (7), we have

\[ R_1(P_m) = a^T u^*(P_m) - \bar{u}(P_m) = 0 \quad (m = 1, \ldots, M_1) \text{,} \]

\[ R_2(P_m) = a^T q^*(P_m) - \bar{q}(P_m) = 0 \quad (m = 1, \ldots, M_2) \text{,} \]

or

\[ a^T u^*(P_m) = \bar{u}(P_m) \quad (m = 1, \ldots, M_1) \text{,} \]

\[ a^T q^*(P_m) = \bar{q}(P_m) \quad (m = 1, \ldots, M_2) \text{.} \]
where \( M_1 \) and \( M_2 \) are the total numbers of the collocation points taken on \( \Gamma_1 \) and \( \Gamma_2 \), respectively. Assembling the above equations, we have

\[
\begin{bmatrix}
    u_{11}^* & u_{12}^* & \cdots & u_{1N}^*
    \\
    u_{21}^* & u_{22}^* & \cdots & u_{2N}^*
    \\
    \vdots & \vdots & & \vdots
    \\
    u_{M1}^* & u_{M2}^* & \cdots & u_{MN}^*
    \\
    q_{11}^* & q_{12}^* & \cdots & q_{1N}^*
    \\
    q_{21}^* & q_{22}^* & \cdots & q_{2N}^*
    \\
    \vdots & \vdots & & \vdots
    \\
    q_{M1}^* & q_{M2}^* & \cdots & q_{MN}^*
\end{bmatrix}
\begin{bmatrix}
    a_1 \\
    a_2 \\
    \vdots \\
    a_N
\end{bmatrix} =
\begin{bmatrix}
    \bar{u}_1 \\
    \bar{u}_2 \\
    \vdots \\
    \bar{u}_M
\end{bmatrix}
\]

(10)

or,

\[
\hat{K}a = \hat{f}
\]

(11)

where \( u_n^*(P_m) \equiv u_{mn}^*, q_n^*(P_m) \equiv q_{mn}^*, \bar{u}(P_m) \equiv \bar{u}_m, \bar{q}(P_m) \equiv \bar{q}_m \).

The coefficient matrix of Eq. (11) is the matrix with \( M \) \((M = M_1 + M_2)\) rows and \( N \) columns. If \( M = N \), it can be solved directly with \( LU \)-decomposition method and if \( M > N \), the least square method is applied to it.

4. Sensitivity Analysis Schemes

4.1. First-order sensitivity analysis

We consider the first-order sensitivities of the potential and the flux with respect to the shape parameter \( \varphi_l \). The potential and the flux at the arbitrary point \( Q \) are approximated by Eqs. (5) and (6), respectively. While \( u^* \) and \( q^* \) are specified on the coordinates of \( Q \), \( a \) is dependent on the profile of the object under consideration and the specified values on the boundary. Direct differentiation of Eqs. (5) and (6) with respect to \( \varphi_l \), we have the approximate expressions of the first-order sensitivities:

\[
\begin{align*}
\dot{u} &= \hat{a}^T u^* \\
\dot{q} &= \hat{a}^T q^*
\end{align*}
\]

(12)

where \( (') \equiv \partial/\partial \varphi_l \). \( \hat{a} \) can be calculated from Eq. (11). Direct differentiation of Eq. (11) with respect to \( \varphi_l \) leads to

\[
\hat{K}a + \hat{K}\dot{a} = \hat{f},
\]

\[
\hat{K}\dot{a} = \hat{f} - \hat{K}a.
\]

(13)

If the specified values on the boundary are not dependent on \( \varphi_l \), \( \hat{f} = 0 \) and therefore,

\[
\hat{K}\dot{a} = -\hat{K}a.
\]

(14)

Equation (13) or (14) is solved for \( \hat{a} \) and then, \( \hat{a} \) is substituted into Eq. (12) to calculate the first-order sensitivities.
4.2. Second-order sensitivity analysis

Differentiating of both sides of Eqs. (12) with respect to $\varphi_k$ again, we have the second-order sensitivities:

\[
\begin{align*}
\dot{u} &= \mathbf{a}^T \mathbf{u}^*, \\
\dot{q} &= \mathbf{a}^T \mathbf{q}^*,
\end{align*}
\]

where $\dot{} \equiv \partial / \partial \varphi_k$. $\dot{a}$ can be calculated from Eq. (13). Differentiation of Eq. (13) with respect to $\varphi_k$ leads to

\[
\begin{align*}
\dot{K}a + \dot{K} \dot{a} + \dot{K} \dot{a} &= \dot{f}, \\
\dot{K} \dot{a} &= \dot{f} - (\dot{K}a + \dot{K} \dot{a} + \dot{K} \dot{a}).
\end{align*}
\]

(16)

If the boundary condition is not dependent on $\varphi_k$, $\dot{f} = 0$ and therefore,

\[
\dot{K} \dot{a} = - (\dot{K}a + \dot{K} \dot{a} + \dot{K} \dot{a}).
\]

(17)

Equation (16) or (17) is solved for $\dot{a}$ and then, $\dot{a}$ is substituted into Eq. (15) to calculate the second-order sensitivities.

5. Computational techniques for accurate solution

5.1. Condition number of coefficient matrix

The T-complete function, as shown in Eq. (4), is the power function of the distance between the origin and the point $r$. The coefficient matrix $K$ becomes near ill-posed as $N$ and $r$ increase. Therefore, in this case, the system of equations can not be solved accurately. For overcoming this difficulty, the following coordinate transformation is applied[28]:

- the object is moved parallel so that the origin is taken on the centroid, and
- the dimensions of the object are scaled up or down so that average of the distances between the collocation points and the origin is unity.

By the above coordinate transformation, the coordinates $(x_i, y_i)$ of the collocation point $P_i$ are transformed as:

\[
\begin{align*}
\dot{x}_i &= \frac{x_i - x_c}{D}, \\
\dot{y}_i &= \frac{y_i - y_c}{D},
\end{align*}
\]

(18)

where $x_c$ and $y_c$ are the coordinates of the centroid on the original coordinates and $D$ is the scaling factor, which are given as:

\[
\begin{align*}
x_c &= \frac{1}{M} \sum_{i=1}^{M} x_i, \\
y_c &= \frac{1}{M} \sum_{i=1}^{M} y_i, \\
D &= \frac{1}{M} \sum_{i=1}^{M} \sqrt{x_i^2 + y_i^2}.
\end{align*}
\]

(19)
5.2. Corner points

The boundary points where the normal vector can not be defined uniquely and where the boundary condition changes are referred to as corner points. In the collocation method, the collocation points are taken on the boundary. Therefore, the placement of the collocation points on the corner points strongly affects the accuracy of solution. This difficulty can be improved by applying “the double collocation points”, which is often employed in the boundary element method using the conforming elements for the same purpose.

The present method employs two kind of double collocation points; the coincident and the nearby double collocation points. In the former, two collocation points are placed on the identical corner point and each collocation point belongs to the different parts of the boundary. In the latter, two collocation points are placed on the individual boundaries adjacent to the corner point. In what follows, the former is employed at

- the points where the boundary condition changes, and
- the geometric corner point on the flux-specified boundary

and the latter at the remaining corner points.

6. NUMERICAL EXAMPLES

6.1. Heat transfer in square plate

A first example is the heat transfer in a square plate (Fig. 1). The boundary conditions are specified as:

\[ q = 0 \quad \text{on segments AB and CD}, \]
\[ u = u_2 = 1 \quad \text{on segment BC}, \]
\[ u = u_1 = 0 \quad \text{on segment DA}. \]

Figure 2 shows the placement of the collocation points for the computation. 44 collocation points are placed uniformly on the whole boundary. 11 collocation points are placed on each segment and then, the coincident double collocation points are on 4 corner points. Besides, 44 T-complete functions are employed for the computation. As the shape parameter for the sensitivity analysis, we take the distance \( L \) between the segments DA and BC.

This example is simple. We, therefore, would like to explain in detail the matrices and the right-hand-side vectors in the initial and the sensitivity analysis processes.
6.1.1. Two-dimensional potential analysis

The collocation points are numbered counterclockwise starting from the point A. Therefore, the collocation points 1 to 11 are taken on AB, the points 12 to 22 on BC, the points 23 to 33 on CD and the points 34 to 44 on DA, respectively. From Eq. (11), we have

\[ \mathbf{a} = \mathbf{K}^{-1} \mathbf{f}, \]

where

\[
\mathbf{K} = \begin{bmatrix}
q_1^* & \cdots & q_{144}^* \\
\vdots & & \vdots \\
q_{11}^* & \cdots & q_{144}^* \\
u_{12}^* & \cdots & u_{144}^* \\
\vdots & & \vdots \\
u_{22}^* & \cdots & u_{244}^* \\
q_{23}^* & \cdots & q_{244}^* \\
\vdots & & \vdots \\
q_{33}^* & \cdots & q_{344}^* \\
u_{34}^* & \cdots & u_{344}^* \\
\vdots & & \vdots \\
u_{44}^* & \cdots & u_{444}^*
\end{bmatrix}, \quad \mathbf{f} = \begin{bmatrix}
\bar{q}_1 \\
\vdots \\
\bar{q}_{11} \\
\bar{u}_{12} \\
\vdots \\
\bar{u}_{22} \\
\bar{q}_{23} \\
\vdots \\
\bar{q}_{33} \\
\bar{u}_{34} \\
\vdots \\
\bar{u}_{44}
\end{bmatrix}.
\]

Equation (20) is substituted into Eqs. (5) and (6). The numerical results are not shown here. They, however, well agree with the theoretical ones[13].
6.1.2. **First-order sensitivity analysis**

$L$ is taken as the shape parameter $\varphi_l$. Since the boundary-specified values are independent of $\varphi_l$, $\dot{f} = 0$. Therefore, from Eq. (14), we have

$$\dot{a} = -K^{-1} \frac{\partial K}{\partial L} a,$$  \hspace{1cm} (22)

where

$$\frac{\partial K}{\partial L} = \begin{bmatrix}
0 & \cdots & 0 \\
\vdots & & \vdots \\
0 & \cdots & 0 \\
\partial u_{12}^*/\partial L & \cdots & \partial u_{12}^*/\partial L \\
\vdots & & \vdots \\
\partial u_{22}^*/\partial L & \cdots & \partial u_{22}^*/\partial L \\
0 & \cdots & 0 \\
\vdots & & \vdots \\
0 & \cdots & 0
\end{bmatrix}.$$  \hspace{1cm} (23)

Equation (22) is substituted into Eq. (12).

Figure 3 shows the numerical results of the first-order sensitivities. The abscissa and the ordinate indicate the sensitivities and the tangential coordinates $t$ starting from the point $A$, respectively. The symbol $\Delta$ denotes the differentiation with respect to the shape parameter and then, the superscript $ex$ the theoretical results. The circles and the triangles indicate the numerical results of $\Delta u$ and $\Delta q$ and then, the solid lines their theoretical ones. The numerical results well agree with the theoretical ones.

![Fig. 3. Distribution of first-order sensitivities](image-url)
6.1.3. Second-order sensitivity analysis

$L$ is taken as the shape parameters $\varphi_l$ and $\varphi_k$. Since $\dot{f} = 0$, from Eq. (17), we have

$$\dot{a} = -K^{-1} \left( \frac{\partial^2 K}{\partial L^2} a + 2 \frac{\partial K}{\partial L} \frac{\partial a}{\partial L} \right),$$

where $\frac{\partial K}{\partial L}$ and $\frac{\partial a}{\partial L}$ are calculated in the first-order sensitivity analysis and then,

$$\frac{\partial^2 K}{\partial L^2} = \begin{bmatrix}
0 & \cdots & 0 \\
\vdots & \ddots & \vdots \\
0 & \cdots & 0 \\
\partial^2 u_{12}/\partial L^2 & \cdots & \partial^2 u_{44}/\partial L^2 \\
\vdots & \ddots & \vdots \\
\partial^2 u_{22}/\partial L^2 & \cdots & \partial^2 u_{22}/\partial L^2 \\
0 & \cdots & 0 \\
\vdots & \ddots & \vdots \\
0 & \cdots & 0
\end{bmatrix}.$$  \hspace{1cm} \text{(25)}

Equation (24) is substituted into Eq. (15).

Figure 4 shows the results of the second-order sensitivities. The circles and the triangles indicate the numerical results and then, the solid lines their theoretical ones. The numerical results well agree with the theoretical ones.

6.2. Heat transfer in thick-walled cylinder

A second example is the heat transfer in a thick-walled cylinder with inner and outer radii $r_1$ and $r_2 (= 3r_1)$, respectively. Considering the symmetry, one-eighth of the cylinder is taken as the domain.
for computation and the specified values on the boundary are (Fig. 5):

\[ u = u_2 = 1 \] on the outer wall,
\[ u = u_1 = 0 \] on the inner wall,
\[ q = 0 \] on the symmetric axes.

The collocation points are placed uniformly on the whole boundary (Fig. 6). Total number of the collocation points are 100; 36 collocation points on the outer wall, 18 on the inner wall and 23 on each symmetric axis, respectively. The coincident double collocation points are placed on 4 corner points. Besides, 100 T-complete functions are employed for the computation. The outer radius \( r_2 \) is considered as the shape parameter for the sensitivity analysis.

6.2.1. First-order sensitivity analysis

Figure 7 shows the results of the first-order sensitivities of the potential \( u \) and its derivative in the \( r \)-direction \( u_r \). The abscissa and the ordinate indicate the sensitivities and the \( r \)-coordinates.
non-dimensionalized by $r_1$, respectively. The circles and the triangles indicate the numerical results of $\Delta u$ and $\Delta u_r$ and then, the solid lines their theoretical ones. The numerical results well agree with the theoretical ones.

**6.2.2. Second-order sensitivity analysis**

Figure 8 shows the results of the second-order sensitivities. The triangles and the circles indicate the numerical results of $\Delta^2 u$ and $\Delta^2 q$ and then, the solid lines their theoretical ones. The numerical results well agree with the theoretical ones.

**7. CONCLUSIONS**

This paper presented the first- and the second-order sensitivity analysis schemes based on the Trefftz method. The physical quantities are approximated by the superposition of the regular T-
complete functions. The expressions of the first- and the second-order sensitivities were derived from the direct differentiation of the original quantities. Since the T-complete functions are not dependent on the shape parameters, the accuracy of the sensitivity analyses is not reduced by the differentiation. Besides, the T-complete functions are regular and therefore, the sensitivities can be estimated more easily than the ordinary boundary element method using the singular fundamental solution. Finally, the present methods were applied to the shape design sensitivity analysis of the two-dimensional potential problems. The numerical results well agree with the theoretical ones. Therefore, we can conclude that the present formulation is verified. By the way, although we consider here the problems with only one design variable as the numerical examples, the present schemes can be easily applied to the problems with more variables. In this case, however, the computational cost may become expensive. For overcoming the difficulty, we now plan to implement the present scheme on the parallel computer systems.

REFERENCES


