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Shape optimization by the boundary element method with a reduced basis reanalysis technique

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Abstract. This paper is concerned with shape optimization problems by the boundary element method (BEM) emphasizing the use of a reduced basis reanalysis technique proposed recently by the author. Problems of this class are conventionally carried out iteratively through an optimizer; a sequential quadratic programming-based optimizer is used in this study. The iterative process produces a succession of intermediate designs. Repeated analyses for the systems associated with these intermediate designs using an exact approach such as the LU decomposition method are time consuming if the order of the systems is large. The newly developed reanalysis technique devised for boundary element systems is utilized to enhance the computational efficiency in the repeated system solvings. Presented numerical examples on optimal shape design problems in electric potential distribution and elasticity show that the new reanalysis technique is capable of speeding up the design process without sacrificing the accuracy of the optimal solutions.

Key words: shape optimization; boundary element method; reduced basis; reanalysis.

1. Introduction

The BEM has become a popular tool in solving problems in both science and engineering. Its main advantage is that for linear problems only discretization of the boundary is required. Thus, meshes can be easily generated and the number of degrees of freedom is often much less than that using a domain-discretized method such as the finite element method or the finite difference method. However, systems discretized by the BEM are usually dense and unsymmetric, whose solvings are time consuming.

Recently, Leu and Mukherjee (1993), Leu (1994), and Wei *et al.* (1994) have carried out optimal shape design for elastic and inelastic problems by the BEM. During an optimization process, the optimal solution is achieved iteratively, where repeated analyses for the intermediate designs are required. Hence, an accurate and efficient reanalysis method is very desirable in that it can speed up the whole design process. The objective of this paper is to employ a boundary element reanalysis technique recently proposed by Leu and Tsai (1995) to enhance the computational efficiency in the repeated systems solvings during the optimization process.

The newly developed reanalysis method for boundary element systems adopted in this study is

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based on a reduced basis formulation. Its efficiency and accuracy in reanalysis problems have been verified in Leu and Tsai (1995). A brief review of the method will be given later. There are few other reanalysis techniques being proposed for boundary element systems as discussed in Leu and Tsai (1995). It is fair to say that the most important goal of any reanalysis technique is its use in design optimization problems to enhance the computational efficiency without sacrificing the accuracy of the optimal solutions. Unfortunately, to the best knowledge of the author, there is no such kind of application being reported in the literature. The present paper is an attempt to bridge this gap.

2. Reduced basis reanalysis method for boundary element systems

This section will briefly review the reduced basis reanalysis method for boundary element systems proposed by Leu and Tsai (1995). For further details and numerical application of the method, the reader is referred to the above reference.

2.1. Statement of reanalysis problem

As described before, an optimal design is obtained through an iterative process. Let's assume that the boundary element system corresponding to the initial design be written as (e.g., Brebbia and Dominguez 1992)

$$\boldsymbol{A}_0 \boldsymbol{x}_0 = \boldsymbol{b}_0 \tag{1}$$

where the system matrix $\boldsymbol{A}_0$ is unsymmetric and is of $n \times n$ (order n); the system unknowns $\boldsymbol{x}_0$ is an $n \times 1$ vector; and the right-hand side $\boldsymbol{b}_0$ is an $n \times 1$ vector. The above system will be referred to as the reference system hereafter.

Direct methods commonly used for solving Eq. (1) include the Gaussian elimination method and the LU decomposition method (e.g., Schwarz 1989). Suppose that the latter method is used, and the system matrix has the following factored form:

$$\boldsymbol{A}_0 = \boldsymbol{L}_0 \boldsymbol{U}_0 \tag{2}$$

where $\boldsymbol{L}_0$ is a lower triangular matrix and $\boldsymbol{U}_0$ is an upper triangular matrix. Having obtained Eq. (2), the unknowns $\boldsymbol{x}_0$ can then be found by a backward followed by a forward substitutions.

During an optimal design process, repeated analyses for the intermediate designs are required. Let the boundary element system for a typical intermediate design be expressed as

$$\boldsymbol{A}\boldsymbol{x} = \boldsymbol{b} \tag{3}$$

This system can also be solved by the Gaussian elimination method or the LU decomposition method, but such a solving is inefficient when the number of unknowns n is large. An approximate but efficient method for solving Eq. (3) will be reviewed in the next subsection.

2.2. Reduced basis reanalysis method

The reduced basis method proposed by Leu and Tsai (1995) for reanalyzing boundary element systems is briefly reviewed in the following.

Let the unknown vector $\boldsymbol{x}$ in Eq. (3) be approximated by

$$x \approx x_a = \Phi c \quad \text{or} \quad x_a = \sum_{i=1}^{s} c_i \phi_i \tag{4}$$

In the above, the subscript "a" indicates that the solution is only approximate, Φ is an $n \times s$ matrix composed of s basis vectors, and c is a column vector composed of the generalized coefficients c_i (i=1, 2, $\cdots$, s).

The basis vectors ϕ_i's are generated as follows. First, premultiply Eq. (3) by A_0^{-1} to yield

$$(I + B)x = \bar{x} \tag{5}$$

where $B \equiv A_0^{-1} \Delta A$, $\Delta A \equiv A - A_0$, $\bar{x} \equiv A_0^{-1} b$. Then, it can be obtained from Eq. (5) that

$$x = (I + B)^{-1} \bar{x} = (I - B + B^2 - B^3 + \cdots)\bar{x} \tag{6}$$

Finally, the terms in the series neglecting the signs are adopted as the basis vectors; namely

$$\Phi = [\phi_1, \phi_2, \phi_3, \cdots] = [\bar{x}\ , B\bar{x}\ , B^2\bar{x}\ , \cdots] \tag{7}$$

Note that the generation of ϕ_i's according to Eq. (7) is computation-inexpensive as explained below. Using the relation $\phi_i = B\phi_{i-1}$ derived from Eq. (7) and the definition of B, one can show that

$$\phi_i = A_0^{-1} \Delta A\, \phi_{i-1} \quad \text{or} \quad A_0 \phi_i = \Delta A\, \phi_{i-1} \qquad (i > 1) \tag{8}$$

As the decomposed form of A_0 has been obtained in Eq. (2), the calculation of ϕ_i, (i>1) only involves the multiplication of ΔA by ϕ_{i-1} followed by a backward and a forward substitutions. Note that ϕ_1 is simply defined as $A_0^{-1} b$, which requires only a forward and a backward substitutions.

By making use of the approximation given in Eq. (4), the reduced system corresponding to Eq. (3) can be derived as follows. Substituting Eqs. (4) into (3) yields the residual vector,

$$R = A\,\Phi c - b \tag{9}$$

If simply let R=0, the resulting system, $A\Phi c$=b, is overdetermined, which cannot be solved directly. In general, the reduced system can be formed by letting the projection of R onto a set of independent vectors ψ_i (i=1, 2, $\cdots$, s) equal zero. This results in

$$\Psi^T A\, \Phi c = \Psi^T b \tag{10}$$

which is equivalent to premultiplying the aforementioned overdetermined system by Ψ^T. Note that Eq. (10) is a system of order s, being usually much smaller than the original one given in Eq. (3). They can be solved by the LU decomposition method. After solving for c from Eq. (10), the approximate solution can be obtained using Eq. (4).

Leu and Tsai (1995) went one step further concerning the above procedure. They proposed a Gram-Schmidt orthonormalization procedure as listed in Table 1 to modify the set of basis vectors ϕ_i's defined by Eq. (7) and to generate another set of vectors ψ_i's such that the new ϕ_i's and ψ_i's satisfy

$$\Psi^T A\, \Phi = I \tag{11}$$

where Ψ is an $n \times s$ matrix composed of ψ_i (i=1, 2, $\cdots$, s) and I is the identity matrix of order s.

Note that in step 2, $\|\cdot\|_1$ represents the L_1 norm. The L_1 norm of a vector is defined as the sum of the absolute value of its components. The normalization performed in step 2 is to make $\|\phi_i\|_1$=1.

Table 1 Gram-Schmidt orthonormalization procedure with respect to A

1.	$\phi_i' = \phi_i - \sum_{k=1}^{i-1} \alpha_k \phi_k$ with $\alpha_k = \psi_k^T A \phi_i$
2.	$\phi_i = \phi_i' / \| \phi_i' \|_1$
3.	$\psi_i = \phi_i$
4.	$\psi_i' = \psi_i - \sum_{k=1}^{i-1} \beta_k \psi_k$ with $\beta_k = \psi_i^T A \phi_k$
5.	$\psi_i = \psi_i' / [\psi_i'^T A \phi_i]$

Other norms can be used also; the L_1 norm, however, is cheaper to calculate.

With the use of the new ϕ_is and ψ_is generated according to Table 1 in forming the reduced system, Eq. (10) becomes the following uncoupled form:

$$c = \Psi^T b \quad \text{or} \quad c_i = \psi_i^T b \quad (i = 1, 2, \cdots, s) \tag{12}$$

where use has been made of Eq. (11). Notice that when one more basis vector, say ϕ_i, is added, only its coefficient c_i needs to be calculated; the previous calculated coefficients c_k (k=1, $\cdots$, $i-1$) remain unchanged.

In applying the above reduced basis method, a common question to be asked is that how many basis vectors should be used to obtain accurate solutions. A computation-inexpensive convergence criterion is:

$$E_c = \frac{|c_s|}{\sum_{i=1}^{s} |c_i|} < e_c \tag{13}$$

where e_c is the error tolerance of E_c. Convergence can be checked by monitoring the value of E_c each time when the number of basis vectors is increased by one. This criterion can be derived as follows. Let's begin with the s-term approximation: $x_a = c_1\phi_1 + c_2\phi_2 + \cdots c_s\phi_s$. It is expected that as x_a converges the contribution of the last term $c_s\phi_s$ to x_a would be very small. Therefore, the number of basis vectors, s, can be chosen such that

$$E_x = \frac{\| c_s \phi_s \|_1}{\| \sum_{k=1}^{s} c_k \phi_k \|_1} < e_x \tag{14}$$

where e_x is the error tolerance of E_x. Since all the ϕ_is have the same L_1 norm of 1 as imposed in step 2 of Table 1, Eq. (14) can be simplified approximately to Eq. (13). Note that according to Leu and Tsai (1995), accurate solutions can be obtained if the tolerance e_c is taken to be 0.01. Therefore, this value will be adopted in all the numerical examples presented later.

3. Reanalysis-based optimal design

In the literature, there are some publications on reanalysis techniques for boundary element systems. However, there is no work on the implementation of such techniques in optimization problems. It is reminded that one important objective of any reanalysis method is to enhance the efficiency of optimal design processes. Thus, the performance of any reanalysis method should not only be evaluated using reanalysis problems, but, more important, also be evaluated using optimization problems. This section discusses how to implement the reduced basis reanalysis method in optimal design problems.

3.1. Optimal design problem and optimizer

A typical nonlinear optimization problem can be posed as follows:

$$\min f(z), \quad z \in R^m \tag{15}$$

subject to

$$h_i(z) = 0 \quad \text{for } i = 1, \cdots, n_e \tag{16}$$

$$g_j(z) \leq 0 \quad \text{for } j = 1, \cdots, n_i \tag{17}$$

$$z_{ll} \leq z_l \leq z_{lu} \quad \text{for } l = 1, \cdots, m \tag{18}$$

where $f(\mathbf{z})$ is the objective function; $\mathbf{z}$ is the design variable vector with m components; h_i and g_j are, respectively, the equality and inequality constraint functions; z_{ll} and z_{lu} are the lower and upper bounds for the design variable z_l; and n_e, and n_i, are, respectively, the numbers of equality constraints and inequality constraints.

In general, an optimal design is achieved in an iterative manner through an optimizer. Typically, an optimizer uses nonlinear programming to propose a new design by providing a better value of the objective function without violating the constraints of a problem. In each design cycle, say the kth step, the input to an optimizer includes z_k, z_{ll}, z_{lu}, $f(z_k)$, $h_i(z_k)$, $g_j(z_k)$, and possibly the gradients of the objective function and constraint functions with respect to z: ∇f, ∇h_i, ∇g_j, also evaluated at z_k. The optimizer then gives a new set of design variables z_{k+1} and also indicates whether the gradients of f, g_j, and h_i are needed in the next design cycle. If the new design is acceptable, the process stops. Otherwise, the iterative process is continued, producing a succession of designs, until an optimal design is obtained.

The optimizer used in this work is called FSQP, which was developed by Zhou and Tits (1994). A brief description of FSQP is given below; further details are available in the above reference. FSQP is a Fortran code for solving constrained nonlinear optimization problems on the basis of sequential quadratic programming. There are two line search algorithms that are implemented in FSQP, among which the Armijo type arch search is chosen in the present work.

3.2. Use of reanalysis technique in an optimal design process

The reanalysis technique reviewed in section 2 finds two applications in the optimal design process discussed above. First, it can be applied to reanalyze the systems corresponding to the intermediate designs. In the whole optimization process, only the analysis for the initial design is performed by the LU decomposition method. Namely, the reference system defined by Eq. (1) is that associated with the initial design. System solvings for all the intermediate designs are carried out by the reanalysis method.

Second, the reanalysis technique can be used to calculate the gradients of the objective function and constraint functions. Typically, the objective function and constraints depend on quantities such as displacements or stresses for elastic problems and are, therefore, implicit as well as explicit functions of the design variables. The gradients of these functions thus cannot be obtained by direct differentiation of these functions with respect to the design variables. In the literature, three approaches have been commonly used for calculating the above gradients: the finite difference approach (FDA), the adjoint structure approach (ASA), and the direct differentiation approach (DDA). For more details on the three methods, the reader is referred to Haug *et al.* (1986). The FDA is convenient to use in conjunction with the reduced basis reanalysis technique to obtain the above gradients, as will be explained below.

The FDA is employed in this study to calculate the gradients of the objective and constraint functions. To this end, m perturbed systems for each intermediate design need to be defined first. Each perturbed system corresponds to the design variables where only one design variable is increased by 0.1 percent of its value from the intermediate design variables, and the other $(m-1)$ design variables remain unchanged. Next, analyses for these m perturbed systems are carried out by the reanalysis method, again with reference to the system associated with the initial design since this is the only system that has been factored. The obtained quantities such as displacements or stresses for each perturbed system can then used to evaluate the objective function and constraints for each perturbed design. Finally, the forward FDA is used to calculate the gradients of the objective function and constraints with respect to each design variable.

4. Numerical examples and discussions

The accuracy and efficiency of the reduced basis reanalysis method have been verified by Leu and Tsai (1995) through several reanalysis problems. Its accuracy and efficiency in shape optimization problems are evaluated here using two example problems; one is an electric potential distribution problem and the other is a thin elastic plate with a cutout subject to biaxial tensions. For all examples, quadratic elements are used. Therefore, the order of boundary element systems, n, equals $2N_e$ for the electric potential distribution problem and $4N_e$ for the elastic plate problem, where N_e is the total number of quadratic elements used. Note that all the computations reported below are carried out on a 486-DX66 personal computer.

4.1. Example 1: electric potential distribution

As depicted in Fig. 1, the problem here concerns electric potential distribution in a circular disk of radius R=1 m with a cutout inside the disk. As is known, such a potential problem is governed by the Laplace equation. The potentials are 100 V (Volts) and 0 V for the inner (cutout) and outer surfaces, respectively. Due to symmetry, only half of the disk is shown and analyzed here. With the x' and y' axes centered at the center of the cutout, a variety of smooth curves (e.g., a circle, an ellipse or a rectangle with rounded corners) can be represented by the equations (Lekhnitski 1968, Sadegh 1988):

$$x' = a(\cos\theta + \eta\cos 3\theta) \tag{19}$$

$$y' = a(\beta\sin\theta - \eta\sin 3\theta) \tag{20}$$

where a controls the size, η the shape, and β the aspect ratio of the cutout. For example, with β=1 the shapes of the cutout for various η's are shown in Fig. 2.

The analytical solution is easy to obtain for the case where the shape of the cutout is a circle, i.e., when β=1 and η=0. Assuming that a=0.4 m, then in this case the exact potential distribution along line AB has the form:

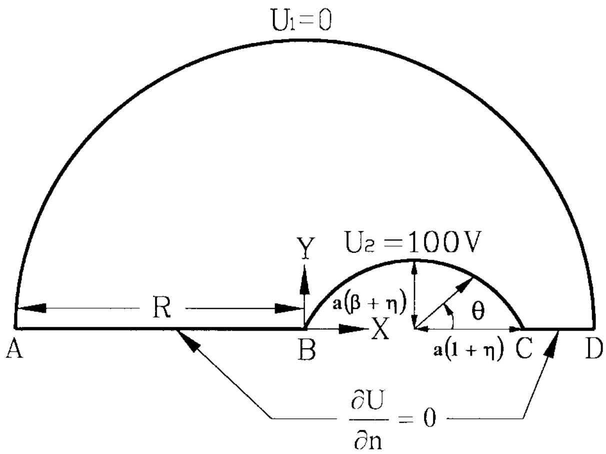

Fig. 1 Electric potential distribution problem

$$U^e(x, 0) = -\frac{100}{\ln 2} \ln \left| \frac{2x-1}{x-2} \right| \tag{21}$$

which can be obtained using conformal mapping. This can be done using the transformation,

$$w(z) = \frac{2z-1}{z-2} \tag{22}$$

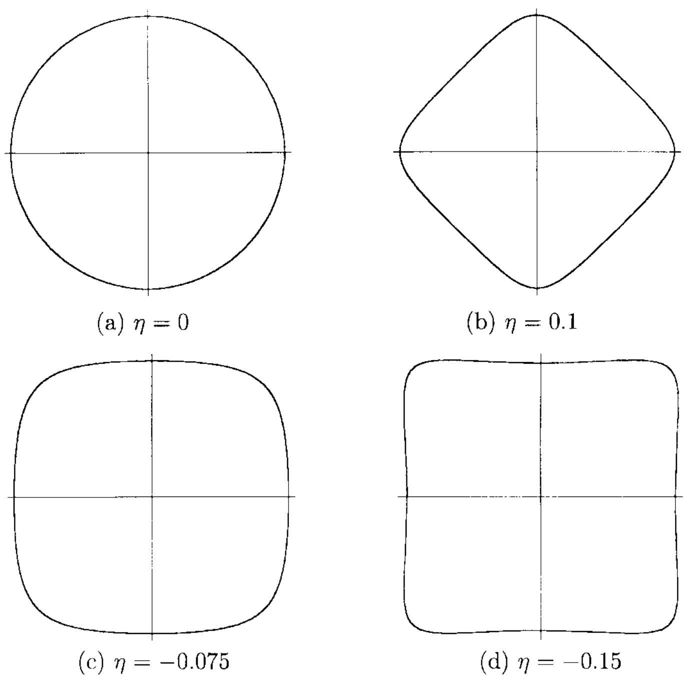

Fig. 2 Shapes of cutout for various η's with β=1

which maps the unit disk $|z|=1$ onto the unit disk $|w|=1$, and maps the cutout $|z-0.4|=0.4$ onto to a concentric disk $|w|=0.5$. The solution in the w-plane can then be obtained easily, which in turn can be used to determine the solution in the z-plane.

Let us take β and η as the design variables. Since the exact solution for the design variables of $\beta=1$ and $\eta=0$ has been given in Eq. (21), an optimal shape design problem can be posed as follows:

$$\min f(x) = \int_{x_A}^{x_B} (U(x,0) - U^e(x,0))^2 dx \tag{23}$$

with the side constraints,

$$0.5 \le \beta \le 1.5 \tag{24}$$

$$-0.15 \le \eta \le 0.1 \tag{25}$$

The ranges for β and η are large enough to allow the shape of the cutout to vary to a large extent. For example, with $\beta=1$, the shapes of the cutout for various η's have been shown in Fig. 2. Concering Eq. (23), the question being asked here is: *For what values of β and η (i.e., shape of the cutout) is the potential distribution along line AB as close as possible to the potential distribution given in Eq. (21)?* Obviously, the optimal solutions for this problem are $\beta=1$ and $\eta=0$, which correspond to U^e. This optimal design problem is somewhat artificial. However, it is still useful for evaluating the accuracy and efficiency of the discussed reanalysis-based optimal design procedure.

Table 2 presents results obtained based on the reduced basis reanalysis method and the LU decomposition method. For the latter results, it means that all the systems for each intermediate design including the one corresponding to that intermediate design and those corresponding to its m perturbed designs are solved by the LU decomposition method. The numbers of elements used for $n=200$ and $n=400$ are 100 and 200, respectively. For the 200-element mesh, there are 38 on AB, 50 on BC, 12 on CD, and 100 on DA. For the 100-element mesh, half of the above elements are used for each side. The elements are uniformly distributed on AB, CD, and DA, and are distributed with an equal θ on BC for both meshes.

The efficiency of the proposed method is clearly seen from Table 2, in which the speed-up is defined as the CPU time using the LU decomposition method divided by that using the reanalysis method. Its accuracy is also acceptable although slightly lower than that using the LU decomposition method. Note that the initial design variables are chosen to be their upper bounds: $\beta=1.5$ and $\eta=0.1$. Let's define N_1 as the number of calculating both the objective function and its gradients and N_2 as the number of calculating only the objective function for the whole optimization process. Then, from Table 2, the proposed method seems to converge faster than the LU decomposition method. This may not be true in general because solutions obtained by the reanalysis method are only approximate. The phenomenon may depend on the optimizer chosen. Since there are two design variables in this problem, the total number of analysis would be $3N_1+N_2$. Therefore, for the proposed procedure, only one analysis is carried out by the LU decomposition method and the other $(3N_1+N_2-1)$ by the reduced basis method. The number of basis vectors, s, required to satisfy the specified error tolerance $e_c=0.01$ of Eq. (13) may be different for the $(3N_1+N_2-1)$ reanalyses. Their average is calculated and also given in Table 2. As can be seen, the averages of s are small for both $n=200$ and 400. This indicates that the basis vectors used are of good quality for approximating the solution for every reanalysis during the whole optimal design process.

Table 2. Optimal solutions for electric potential distribution

		Present	LU	Speed-up
Order n=200	CPU (sec)	405.57	588.97	1.45
	Optimal (β, η)	(1.0226, −0.0234)	(0.9992, 0.0004)	
	(N_1, N_2)†	(8, 9)	(10, 10)	
	Average $s^\ddagger$	4.03		
Order n=400	CPU (sec)	2225.69	4326.48	1.94
	Optimal (β, η)	(0.9942, −0.0110)	(0.9964, 0.0003)	
	(N_1, N_2)	(10, 12)	(11, 16)	
	Average s	4.49		

$^\dagger N_1$=number of calculating both the objective function and its gradients
$^\dagger N_2$=number of calculating only the objective function
$^\ddagger s$=number of basis vectors used

4.2. Example 2: Elastic plate with cutout

Consider a thin square plate with a cutout in the center. Due to symmetry, only one quarter of the plate needs to be modeled, which is shown is Fig. 3. The shape of the cutout is again described by Eqs. (19) and (20), and β and η are again treated as the design variables. The plate is subjected to biaxial tensions t_x=5MPa and t_y=6MPa under plane stress condition. Other data are as follows: a=1 m, L=10 m, Young's modulus E=200 GPa, and Poisson's ratio ν=0.25.

Two meshes are considered, one with 50 elements and the other with 100 elements; their orders are 200 and 400, respectively. For the 50- and 100-element meshes, there are, respectively, 10 and 20 elements on each of the five sides, including the cutout. The elements along each straight side are uniformly distributed and the elements along the cutout are distributed with an equal θ angle.

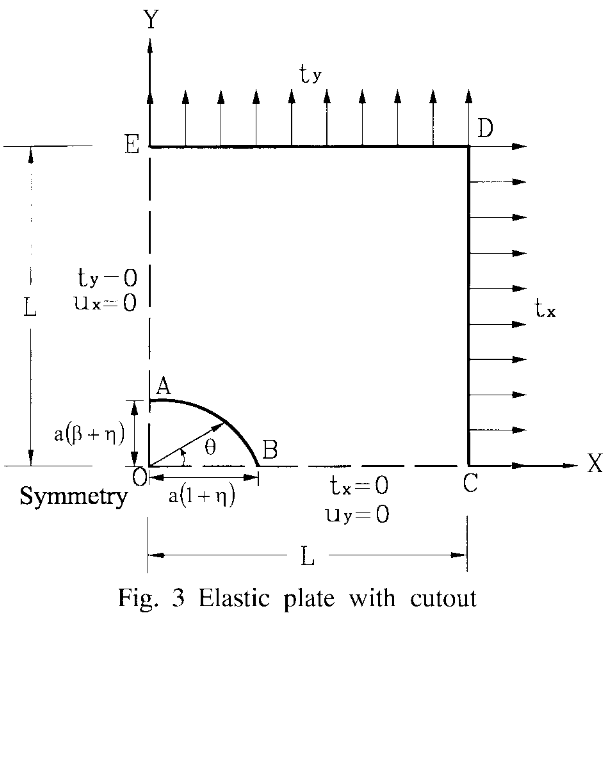

Fig. 3 Elastic plate with cutout

Two optimal design problems are investigated for the thin plate example. Both aims to minimize the objective function,

$$f = \frac{1}{L_c} \int_{\partial B_c} (\sigma_t(S) - \bar{\sigma}_t)^2 dS \tag{26}$$

where ∂B_c is the cutout boundary, σ_t is the tangential stress on ∂B_c, $\bar{\sigma}_t$ is the mean value of σ_t, and L_c is the length of ∂B_c. The meaning of minimizing f is to require the tangential stress on the cutout to be as uniform as possible.

In the first design problem, β is chosen as the single design variable with $0.5 \leq \beta \leq 2$ and for a fixed η=0. In the second design problem, η is chosen as the single design variable with $-0.15 \leq \eta \leq 0.1$ and for a fixed β=1.2. The theoretical optimal solution for both design problems is (β, η)=(1.2, 0). In this case, the shape of the cutout is an ellipse, i.e., η=0, with the lengths of the axes being 1 m and 1.2 m along the x and y axes, respectively. The above solution can be found in Timoshenko and Goodier (1970). Assuming an infinite plate, they showed that for an elliptical cutout with a and b being the lengths of the axes along the x and y axes, if

$$\frac{t_y}{t_x} = \frac{b}{a} \tag{27}$$

then the tangential stress σ_t will be uniform and its value equal $t_x + t_y$. As t_x=5MPa, t_y=6MPa, and a=1 m are used, the optimal value of b will be 1.2 m; therefore the optimal $\beta=a/b$=1.2. Tables 3 and

Table 3. Optimal solutions for elastic plate: Initial β=0.5

		Present	LU	Speed-up
Order n=200	CPU (sec)	92.98	166.15	1.79
	Optimal (β)	1.186	1.178	
	(N_1, N_2)	(4, 2)	(4, 4)	
	Average s	3.56		
Order n=400	CPU (sec)	420.02	1111.42	2.65
	Optimal (β)	1.176	1.183	
	(N_1, N_2)	(4, 2)	(4, 4)	
	Average s	3.56		

Theoretical optimal β=1.2

Table 4 Optimal solutions for elastic plate: Initial η=0.1

		Present	LU	Speed-up
Order n=200	CPU (sec)	46.57	68.71	1.48
	Optimal (η)	−0.025	0.025	
	(N_1, N_2)	(2, 1)	(2, 1)	
	Average s	2.75		
Order n=400	CPU (sec)	223.16	459.84	2.06
	Optimal (η)	−0.025	0.025	
	(N_1, N_2)	(2, 1)	(2, 1)	
	Average s	2.5		

Theoretical optimal η=0

4 present results for these two design problems. Again, the efficiency and accuracy of the reduced basis reanalysis method in optimal design problems is verified.

5. Conclusions

This paper has attempted shape optimization problems by the BEM using a newly developed reanalysis technique. The reanalysis method is based on a reduced basis formulation. There are several merits with the method. In particular, the reduced system has been uncoupled through an orthonormalization procedure; this results in a computation-inexpensive convergence criterion for deciding adaptively the required number of basis vectors. Such an automatic determination is very desirable since the required number of basis vectors will vary according to how much the design changes during an optimal design process.

Implementation of the reduced basis reanalysis method in an optimal design process has been discussed in detail in this paper. In such a process, the reanalysis method is mainly used for solving efficiently the boundary element systems encountered. Presented example problems on shape optimization demonstrate that the new reanalysis technique does enhance the efficiency of an optimal design process without losing the accuracy of the optimal solutions.

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