

Boundary Elements and a Green's Function Library

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1 Introduction

The boundary element method (BEM) is now an established procedure for obtaining numerical solutions for a variety of problems in engineering and applied mathematics. The formulation of the BEM relies heavily on the existence of suitable Green's functions. Indeed, Green's functions are the BEM's main analytical ingredient.

With the conventional BEM, a significant analytical step is taken at the outset, and this involves only the *simplest* Green's functions. The result is a representation integral for desired fields in terms of *boundary values* of the fields. This result is obtained before elements and approximations of any kind are introduced. Unfortunately, when only the simplest Green's functions are used, about half of the boundary values of the fields are unknown in the representation integral at this stage. Elements and approximations are needed afterwards, in essence, to numerically solve a boundary integral equation. This is done to obtain the mentioned unknown boundary data. Then, with all boundary data known, the representation integral provides the desired field solution throughout the region of interest. The process, in effect, reduces a three-dimensional problem to a two-dimensional one. This is one of the great features of the BEM.

Now if *more sophisticated* region-specific Green's functions were to be used at the outset, less unknown boundary data would appear in the representation integral, fewer elements and associated approximations would be needed with the BEM, and accuracy could be increased while computing demands would be reduced. Carrying such reasoning to its end, one would need no elements at all if exact, region-specific Green's functions could be found. No unknown boundary data would appear in the representation integral in such cases, and they would provide the desired fields everywhere after the first step. Errors for real problems would be limited to numerical quadrature errors on integrals with known integrands.

The *simplest* Green's functions (G) which give fields due to point disturbances in all of space, are well-known in analytically-convenient, closed form for broad classes of problems. The more advantageous, *more sophisticated* Green's functions (G^*), which give such fields in the presence of bounding surfaces and other problem-specific features, have not been known, in any form, except for relatively few simple geometries and boundary conditions. Indeed, this is perhaps the main reason why the conventional BEM is based on the simplest functions, despite considerable computational effort in using it for industrial problems.

However, there has been some recent success in constructing more sophisticated Green's functions G^* , in analytical or approximate-analytical form, for specific shapes S , for a variety of classes of problems e.g.

[1]. Therefore, one might try to preserve many of the mentioned advantages with the BEM, when G^* is known analytically, by first assembling a 'library' of such existing G^* . Then simplified computer codes, which could be nothing more than quadrature routines involving prescribed boundary data and the G^* for specific S , could be written by users to solve their own real problems. In fact, many such codes already

exist as "the last step" of existing BEM codes. With a library of G^* , the last step is all that would be required for many problems. Successful experience with such a library could be motivation to construct more and more sophisticated G^* entries over time.

Despite this scenario, it is clear that many classes of problems, for many geometrical shapes, will probably defy, indefinitely, the construction of G^* in even an approximate-analytical form. For such cases it is possible to construct G^* in *discretized* or *numerical* form, for a variety of difficult but commonly occurring surfaces S . These G^* could be placed in another type of library. Such library entries would take time and computational effort to create. However, like the creation of analytical G^* , these would be one-time tasks. With modern technology for storage and quick retrieval of massive amounts of data, e.g., on compact disk, and transmission of such data on computer networks, it is possible to take a fresh look at the advantages of using even numerical G^* , versus conventional BEM which uses the simpler analytical G .

How to construct a library of discretized G^* , which would consist of matrices of numbers as its main ingredient, and how to use the library, are less clear than with analytical G^* ; but these matters are the subject of this paper. In fact, the conventional BEM is a prime vehicle for constructing discretized G^* . We intend to show that use of discretized G^* , with some attention to standardized protocol, could be almost as convenient and accurate for problem solving as having their analytical or approximate-analytical counterparts. Speed might be improved too. To obtain discretized G^* for the two-surface problem, as described below, requires a number of matrix multiplications. This can take some time. However, existing G^* in analytical form often require extensive integrations or series summations, and these are notorious in the amount of time and effort to get numerical values from them.

The focus of the rest of this paper is to look in some detail at the consequences of getting *more sophisticated Green's functions* G^* into the *BEM picture*. To fix ideas, we outline the essential aspects of creating a library of discretized or numerical Green's functions for problems of scattering of time-harmonic acoustic fields by one or more three-dimensional obstacles, each bounded by a smooth surface S . Ideas for one and two scatterers are treated explicitly. How to deal with more than two scatterers will be obvious, and simplifications which occur whenever G^* is known in at least approximate-analytical form will be apparent. How to proceed for problems other than ones in acoustics, such as elastostatics, time-harmonic elastodynamics, steady state heat conduction, or any problems governed by linear elliptic partial differential equations, should be apparent as well.

Nevertheless, the NIST workshop, which gave rise to these proceedings, was concerned with ***Green's functions and boundary elements with applications for modeling the mechanical behavior of advanced materials***. Thus we close this introduction with some comments on the kind and character of G^* useful for this purpose.

Specifically, for materials-related problems, we wish to create for the library as many *Greens functions* G^* as possible, which contain the *geometrical and constitutive features of the most important advanced materials*. Fields of greatest interest are likely to be elastostatic or elastodynamic, when modeling mechanical behavior; but again, acoustic, thermal, or even electromagnetic responses to certain inputs may be relevant to such behavior.

A typical strategy would be to model generic or model problems for "cells" of composite materials, first for materials in their perfectly-bonded, *undamaged* state. Then, the G^* , in either analytical or discretized form, for these problems could be formed and stored in the library, ready for nominal, representative, static loads to be applied by materials analysts. From these loads and library of G^* , a variety of responses could be easily calculated from which, in turn, a "cell" stiffness or modulus could be constructed. Macrostructural behavior of bodies made of such composites could thereby be assessed.

Subsequent models could include *damaged* materials, i.e., those with common disbonds in advanced composites or cracks which grow in characteristic patterns. Then, library entries G^* , with the essential, difficult, geometrical features of these models, could be created, ready for scientists to assess the

influence of the damage on local stiffness and thus, subsequently, on the macrostructural behavior of bodies containing such defects. In any case, with a library of proper G^* , the desired fields may be generated by representation integrals similar to the ones discussed above. The value of "what-if" experiments, that could be quickly and easily run with a good library of G^* for complex materials, damaged or undamaged, would evidently be considerable.

2 The one-surface problem

Consider time-harmonic scattering of acoustic waves in 3-D by a bounded body B' with surface S . The representation integral for the acoustic field u at a point P in B exterior to B' is

$$2u(P) = \int_S \left[\frac{\nabla u(q)}{\nabla n} G(q, P) - u(q) \frac{\nabla}{\nabla n} G(q, P) \right] dS_q \quad (1)$$

where $G(P, Q) = G(Q, P) = -e^{ikR}/(2\pi R)$, R is $|Q - P|$, with point Q also in B and points q (and p et seq.) on S , k is a frequency parameter, and u satisfies a radiation condition at infinity. Representation (1) is obtained by applying Green's theorem to u and G in the usual fashion [2]. Now if $\nabla u(q)/\nabla n = f(q)$ is prescribed on S , expression (1) does not give the solution for $u(P)$ since $u(q)$ is unknown.

However, suppose $G^* = G + w$, where w is a regular function (satisfying the same governing differential equation as u), can be found, and G^* used in place of G , such that

$$\frac{\nabla}{\nabla n_q} G^*(q, P) = 0 \quad \text{for } q \in S, \quad (2)$$

then (1) reduces to the integral

$$2u(P) = \int_S f(q) G^*(q, P) dS_q \equiv S_0^* f \quad (3)$$

which gives, in fact, the solution $u(P)$ or $u(p)$. With G^* instead of G , everything under the integral sign is known.

Thus with known G^* for given S and k , it is clear that solutions for arbitrary f are obtainable with a simple quadrature. Having a library of G^* 's, for as many shapes S as possible, would therefore have obvious advantages.

Alternatively, consider the limit as P goes to p in (1). The result is

$$u(p) + \int_S u(q) \frac{\nabla}{\nabla n_q} G(q, p) dS_q = \int_S f(q) G(q, p) dS_q \quad (4)$$

or in operator form

$$Au = S_0 f. \quad (5)$$

Therefore in light of (3) and (5) it is true that on S

$$A^{-1}S_0 = \frac{1}{2} S_0^*, \quad (6)$$

such that solving the boundary integral equation (BIE) (4), is formally equivalent to finding the Green's function G^* (cf. [3], and [4] eqs. (28), (29)).

Pursuing this line of reasoning a bit further, it can be shown [2], by applying Green's theorem to G and G^* , that G^* satisfies the BIE (4), with $2G$ in place of the integral on the right hand side of (4). Since this is true, it follows that

$$G^*(q, P) = 2A^{-1}G(q, P), \quad (7)$$

where it is important to note that relation (7) between G and G^* holds so long as at least one point in the argument of each function is on S. Formally inserting expression (7) for G^* into (3) we obtain

$$u(P) = \int_S f(q) A^{-1}G(q, P) dS(q). \quad (8)$$

If A^{-1} is assumed known, (8) like (3), represents the solution $u(P)$. Equation (8) is hardly a new result. Nevertheless, its use as considered below does appear to be new.

With existing boundary element methodology, it is possible to regard (8) as having many of the advantages of (3). Specifically, it is possible to first form a nodal-value-approximation to A^{-1} , say $\boxed{A_N^{-1}}$, in the form of a (NxN, (N=number of nodes)) matrix, for as many shapes S and frequencies k as desired, using a good robust BEM. Next, multiply $\boxed{A_N^{-1}}$ by G evaluated at nodes q for chosen P . We now have a nodal approximation to $G^*/2$. Now improve this approximation over the boundary elements using appropriate shape functions in the variable q . Similarly represent f , so that it is now possible to integrate the only remaining variables under the integral in (8), namely, products of shape functions. The result of this integration is another square (NxN) matrix K , similar in character to the stiffness matrix in finite elements. With this process, an approximate form of (8) may be written (sum on $i, j = 1 \dots N$)

$$u(P) = f(l_i) A_K^{-1}(l_i, q_j) G(q_j, P) \quad (9)$$

where $f(l_i)$ is a (1xN) row matrix of nodal values of f , $G(q_j, P)$ is the (Nx1) column matrix of nodal values of G for desired (parameter) P , and $A_K^{-1}(l_i, q_j)$ is the product of A_N^{-1} with K .

The ingredients in (9) and the strategy surrounding their formation and use deserve more discussion.

Suppose a library of A_N^{-1} were available for a sequence of (say oblate) spheroidal-shaped rigid scatterers in an acoustic medium. Let the entries be specified by an eccentricity parameter e and frequency parameter k . Now a library user, with known f 's in hand (i.e. known input waves at a certain k), would like to know the scattered field at desired P , from a rigid spheroid of certain e . This user could proceed as follows.

Locate the proper A_N^{-1} for chosen e and k , specify f in a standard (easy) format, and specify a list of specific P locations for the desired fields. The software to pick the necessary A_N^{-1} from the library, multiply by K to get A_K^{-1} (i.e. do the integration in (8)), and finally do the multiplications in (9) with the row f and column of G for chosen P , could all be part of a black box. The box itself could be part of the library. The point is, with a good library, accurate reliable $u(P)$ values could be obtained rather quickly with little or no knowledge of the underlying process required from the user.

In fact, if a quadrature scheme (order of shape functions, etc.) could be decided upon in advance, it would be possible to store A_K^{-1} rather than A_N^{-1} , and save some execution time. This and other such issues should be transparent to the user. In any case, interested knowledgeable users, who might wish to write some of their own library-access software, are faced primarily with tasks involving formation and multiplication of matrices. The main, complex, time-consuming task of getting A_K^{-1} would already have been done.

3 The two-surface problem

In this section we consider the same scattering problem as in section 2 but with two bounded scatterers. For now, consider their surfaces, S_1 and S_2 to be disjoint; other configurations will be treated later. Here, we assume the desired scattered fields satisfy a radiation condition as before and also satisfy the boundary conditions

$$\frac{\int u}{\int n} = f_j \quad j = 1, 2 \quad (10)$$

where f_1 and f_2 are given functions on S_j .

Proceeding as in section 2, the counterpart of equation (1) for the two surface problem is

$$\begin{aligned} 2u(P) = & \int_{S_1} [f_1(q_1)G(q_1, P) - u(q_1)\frac{\int G(q_1, P)}{\int n_q}]dS_q \\ & + \int_{S_2} [f_2(q_2)G(q_2, P) - u(q_2)\frac{\int G(q_2, P)}{\int n_q}]dS_q \end{aligned} \quad (11)$$

Again, (11) contains unknown data on the surfaces, namely, $u(q_1)$ and $u(q_2)$ on S_1 and S_2 , respectively.

However if G^* for S_2 were known and used in place of G in (11), i.e., where

$$\frac{\int G^*(q_2, P)}{\int n_q} = 0, \quad (12)$$

then (11) reduces to

$$2u(P) = \int_{S_1} [f_1(q_1)G^*(q_1, P) - u(q_1)\frac{\int G^*(q_1, P)}{\int n_q}]dS_q + \int_{S_2} f_2(q_2)G^*(q_2, P)dS_q \quad (13)$$

which is the two-surface counterpart of (3) with G^* for S_2 . Note the dependence on the unknown function $u(q_2)$ is missing, such that the integral over S_2 is known. Of course $u(q_1)$, unknown on S_1 , is still present.

To simplify the subsequent discussion, assume further that f_2 is zero. (It is a simple matter conceptually to add this integral back for nonzero f_2 , and dealing with this term is no more difficult than with (3) via (9)). Without the last integral, (13) is formally the same as (1), with G^* in place of G .

One might be tempted now to try to replace G^* in (13) with a function G^{**} , say, where the normal derivative of G^{**} vanishes, not only on S_2 , as does G^* , but also on S_1 . With such a G^{**} , an equation like (3) could be written. Then, in principle, the strategy described above following (3) would pertain. However, there is difficulty enough in trying to find analytical G^* or numerical G^* as described for the one-surface problem, such that a comparable strategy for a G^{**} is best postponed, perhaps indefinitely.

Nevertheless, it is worthwhile to view (13) in a fashion similar to (1), with (4), and (5). That is, imagine solving a BIE like (5) for u on S_1 where only S_1 needs be discretized with boundary elements. This is possible, without discretizing S_2 , if G^* is used in the process. Information about S_2 is contained in G^* . Thus, with G^* , the two surface problem, via the BIE/BEM, is formally no more difficult than the one surface problem.

If one must use a numerical G^* in (13), many of the issues already addressed in connection with (7), (8), and (9) are still applicable. However, there are some new issues as well.

Specifically, note first that the arguments of G^* and its normal derivative as appear in (13) involve q_1 as well as P . Thus any BIE/BEM methodology involving S_1 , and subsequent use of (13) as a solution for $u(P)$, requires G^* as a two-point function, where neither point is on S_2 . Thus (7) is insufficient for this purpose.

In light of this, consider another consequence of applying Green's theorem to G and G^* , namely (cf. [5], [6]),

$$2 G^* (Q, P) = 2 G(P, Q) - \int_s G^* (l, P) \frac{\mathcal{I}}{\mathcal{I}n_l} G(l, Q) dS_l \quad (14)$$

where S in (14) should be regarded as S_2 . Now since l in the argument of G^* in (14) is on S_2 , we may use (7) to write (14) as

$$G^* (Q, P) = G(Q, P) - \int_s \frac{\mathcal{I}}{\mathcal{I}n_l} G(l, Q) A^{-1} G(l, P) dS_l, \quad (15)$$

where Q and P may be interchanged in any of these expressions, since both G and G^* are symmetric in these variables. Similarly, (cf. [2]) it is true that

$$\frac{\mathcal{I}}{\mathcal{I}n_{q_1}} G^* (q_1, P) = \frac{\mathcal{I}}{\mathcal{I}n_{q_1}} G(q_1, P) - \int_s \frac{\mathcal{I}}{\mathcal{I}n_l} G(P, l) A^{-1} \frac{\mathcal{I}}{\mathcal{I}n_{q_1}} G(l, q_1) dS_l \quad (16)$$

where again integrals over S mean over S_2 .

Now with (15) and (16), and existing boundary element methodology, the reasoning leading to a library of information about S_2 is similar to that surrounding (8). Specifically, it is possible to write (15) as

$$G^*(Q, P) = G(Q, P) - G^{n_l}(Q, l_i) A_K^{-1}(l_i, q_j) G(q_j, P) \quad (17)$$

where the n superscript means normal derivative at l , and l_i and q_j are the arguments for row and column matrices as before, and $A_K^{-1}(l_i, q_j)$, is exactly the same matrix encountered earlier. A similar expression exists for the normal derivatives in (16), namely,

$$G^{*n_q}(Q, P) = G^{n_q}(Q, P) - G^{n_l}(P, l_i) A_K^{-1}(l_i, q_j) G^{n_q}(q_j, Q) \quad (18)$$

Note that a row-times-square-times-column multiplication is required for each P, Q choice in expressions (17) and (18). The results of such operations are the G^* function evaluations as needed in a BIE/BEM treatment of the surface S_1 . Other aspects of the treatment are the same as if the free-space G were usable, i.e., as if S_2 were not present.

Observe that expressions (15) and (17) have the classic form for a region-dependent Green's function, i.e., $G^* = G + w$, where (minus) the integral term in (15) is w , and (minus) the triple-matrix product in (17) is (an approximate) w . Moreover, each expression for G^* can be interpreted as "the field at Q due to a point disturbance at P in the presence of a surface ($S=S_2$) on which the normal derivative of the field vanishes". This is precisely the interpretation of (one of a class of) region dependent Green's functions.

4 Partitioning

Consider equation (11) again (with f_2 zero), and suppose limits are taken as P goes to p_1 on S_1 and p_2 on S_2 , respectively. The result is

$$A_{11} u_1 + A_{12} u_2 = S_{11} f_1 \quad (19)$$

$$A_{21} u_1 + A_{22} u_2 = S_{21} f_1 \quad (20)$$

where the operator notation of (5) is invoked with the following additional considerations: the first subscript on the A and S operators refers to p_i locations on S_i , whereas the second subscript on those operators refers to q_j locations on S_j ; the single subscript on u and f refers to q_j locations on S_j ; for the A_{ij} operators with i not equal to j , the free $u(p)$ term (cf. (4)) is zero.

Now if u_2 is formally eliminated from (19) and (20), the result is

$$(A_{11} - A_{12} A_{22}^{-1} A_{21}) u_1 = (S_{11} - A_{12} A_{22}^{-1} S_{21}) f_1. \quad (21)$$

Next, if the group of terms in parentheses on the left side of (21) is called A^* , and the group of terms in parentheses on the right side is called S^* , (21) is formally the same as (5). Thus the presence of S_2 is manifest in the operator-triple-products with A_{22}^{-1} in their centers.

In light of the observations about (21), made possible by the partitioning process, and the form of equations (1) and (13) [with f_2 zero], and the form of equations (15) and (16) [or (17) and (18)], it probably occurs to the reader to question whether the partitioning process and the process of defining and using G^* are equivalent. Indeed, this is the case as is rigorously shown in [2].

Specifically, if G^* and its normal derivative, as given by (15) and (16), are used in place of G and its normal derivative in (4), the " $_{11}$ " terms in (21) come from the " G " part of the Green's function, and the triple-product terms come from the " w " (integral (over S_2)) part.

Note finally that the surfaces S_1 and S_2 above need not be disjoint. The partitioning of a single surface into two parts is arbitrary and really a matter of convenience. For example, S_2 may be a common-shaped appendage on a variety of problem-specific shapes S_1 . Specifically, S_2 may be a thin antenna attached to the surfaces S_1 of different vehicles. Most of the discussion in sections 3 and 4 applies in such cases.

5 Discussion

Consider again the work involved in the creation and use of the Green's function library. For clarity, consider these matters for the one- and two- surface problems separately.

For the one-surface problem, the suggested strategy is to form a library of A_K^{-1} for single surfaces S , dependent on shape parameters, and for material parameters characterizing common acoustic media. The desired field for a particular S and k would then be given by (9). Of course it would take time and effort using existing BEM to form A_K^{-1} . However, we believe that ease and speed of subsequently obtaining scattered fields, using A_K^{-1} from the library, would more than justify the creation of individual entries. This has certainly been the case in our experience with the small library we have already created for our own use. Like any library, the larger the better, but creation costs would suggest some advance determination of parameters characterizing those A_K^{-1} which would be used repeatedly. The number of entries for acoustic scattering would probably be more a function of the variety of shapes rather than the number of different acoustic media. The size of the individual entries would be a function of the degrees of freedom, or number of nodes N in the BEM used to get the A_K^{-1} . In any case, all of the work to get A_K^{-1} would be done in advance of their use by the library formers.

For the users, the time to get $u(P)$ via (9) would depend primarily on N . The user specifies f , and picks the particular A_K^{-1} needed, then $f(l_j)$ would be formed by library software. Next, the software would multiply $f(l_j)$ by $A_K^{-1}(l_j, q_j)$ to get a row dependent on q_j . Subsequent operations by the same software to get u would involve "(1xN) row times (Nx1) column" operations for each (perhaps many) P from a list of P specified by the user. A new multiplication involving the (NxN) $A_K^{-1}(l_j, q_j)$ would be required only for new f .

For the two-surface problem the situation is a bit more complicated and more computationally intensive. Here, the strategy is to set up and solve the BIE equivalent of (4) or (5) wherein only S_1 needs be discretized. For this, as already noted, G^* replaces G . In principle then, solving the two-surface problem using G^* is formally identical to solving the one-surface problem via the conventional BEM using G . However, to actually implement this formality, both $G^*(p_1, q_1)$ and its normal derivative at q_1 are required, where neither p_1 nor q_1 are on S_2 . Then, to finally get $u(P)$ via (13), one needs $G^*(P, q_1)$ and its normal derivative at q_1 . Again, neither point is on S_2 .

Getting the values of G and its normal derivative at the mentioned points is easy, but getting the corresponding values of G^* and its normal derivative at the same points requires (17) and (18). (Expression (7) is insufficient since $q=q_1$ is required). Thus, just to obtain values of the required Green's functions at points off of S_2 , more matrix multiplications via (17) and (18) are needed than to get $u(P)$ via

(9), for the *one-surface problem*. Then, after obtaining those values, there still remains the job of using them to set up the BIE (5), solving (5), and finally using (13) to get $u(P)$ for the *two-surface problem*.

Nevertheless, despite the number of steps, there is considerable conceptual and strategic advantage in utilizing a library-collection of A_K^{-1} for the two-surface problem, as well as for the one-surface problem. Matrix multiplications are the main computational burden in (17) and (18). However, such are less formidable than discretizing a commonly-occurring but complex shape S_2 each time - not to mention that the operator (matrix) A^* which needs to be inverted is smaller than the A (for the union of S_1 and S_2) when only G is used.

With the library in place, this, in a nutshell, is the tradeoff: *less user expertise and modeling effort plus certain CPU time required to solve a problem using G^* , versus less of the first two items, and probably less CPU too, than when using G* . We believe in the long run this is a good trade.

In any case, having a library of G^* , in analytical or discretized form, the BEM should become a more powerful, more accurate and even a faster tool, which would be usable on smaller computers, by less-expert users.

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