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Improved Extrapolation Technique in the Boundary Element Method to Find the Capacitances of the Unit Square and Cube

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Extrapolation of the number N of subdivisions to infinity in the boundary element method involves fitting computed results to a polynomial in $1/N$. A technique of choosing the sizes of the subdivisions in such a way that the terms of lowest order in $1/N$ are eliminated, giving a more accurate extrapolation, is described. The technique is used to establish the capacitances of the unit square and cube with relative errors of 3×10^{-7} and 3×10^{-6} respectively.

1. INTRODUCTION

The boundary element method (BEM), also known by the generic name integral equation method, has been used in many fields, including that of electrostatics, where it is sometimes referred to by the specific names boundary charge, surface charge, or charge density method. In all these manifestations the accuracy of a result depends on the total number N of boundary segments that are used. Clearly it would be desirable to be able to extrapolate the effective value of N to infinity, but it seems that at present there is very little theoretical knowledge about the asymptotic dependence of the discretization error of the BEM [1]. The purpose of the present paper is therefore to describe an efficient empirical technique for extrapolating N to infinity. Three problems in electrostatics will be used to illustrate the technique, which can also be applied to other types of problems that have a kernel of the same form.

In electrostatics the BEM is sometimes used to find capacitances and more frequently to solve Laplace's equation for systems of electrodes, usually in order to integrate trajectories of charged particles through the system [2]. The first use of the BEM to calculate a capacitance seems to be that of Maxwell [3, 4], who used it in 1878 to find the capacitance of a thin square plate with sides of unit length, subdividing the plate into 36 square segments. The BEM remains the most appropriate method for calculating this capacitance, since it seems that an analytic solution still does not exist. This is true also for the capacitance of the unit cube. The technique to be described will be used to find these two capacitances to a higher accuracy than ever before. The technique is of course also relevant to the use of the BEM in solving a wide range of other electrostatic and related problems.

2. SOURCES OF ERROR IN CALCULATING A CAPACITANCE

We start with a problem that has a known solution, the capacitance of a flat circular disc of zero thickness and radius r, which is $8\varepsilon_0 r$ [5]. We will look empirically at the way in which the calculated capacitance depends on the number and size of subdivisions and will then consider the possible reason for the observed behaviour.

In most versions of the BEM in electrostatics the electrodes of a system are subdivided into segments and the surface charge density σ on each segment is taken to be uniform, on the assumption that the segments have been chosen to be sufficiently small. This represents the only approximation made in the BEM. The column vectors of segment voltages $\mathbf{V}$ and their surface charges $\mathbf{Q}$ are related through the matrix $\mathbf{A}$,

$$\mathbf{V} = \mathbf{AQ}, \tag{1}$$

where the elements A_{ij} of $\mathbf{A}$ represent the potential at the midpoint of segment i due to a unit charge that is uniformly distributed on segment j (and it is assumed here that there are no space charges present). Inversion of $\mathbf{A}$ leads to the individual segment charges Q_j, and then the capacitance C of the system is given by the sum of the Q_j, over the appropriate segments and for the appropriate set of voltages.

In the present problem the disc of radius R is subdivided into annular segments $j(= 1 \text{ to } N)$ that are bounded by the radii r_{j-1} and r_j. These radii can be uniformly spaced in the interval 0 to R, but we will use a more general distribution of the form

$$r_j = R(1 - (j/N)^m) \tag{2}$$

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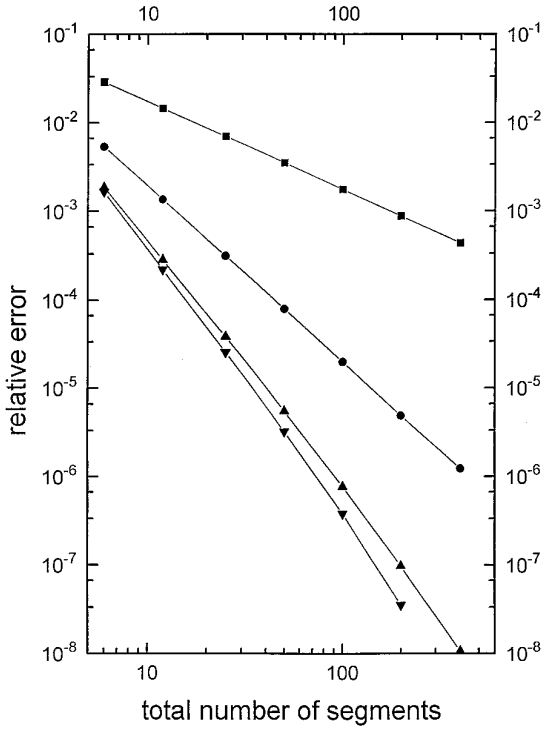

FIG. 1. Dependence of the relative error of the capacitance of a disc on the total number of segments, for the four types of segment distributions characterized by $m = 1$ to 4 (see text): (■) $m = 1$; (●) $m = 2$; (▲) $m = 3$; (▼) $m = 4$.

and will consider values of m from 1 to 4. As the value of m increases the segments near the rim of the disc become progressively narrower than those near the centre. An example of a distribution with $m = 2$ will be given later (see Fig. 2). The program CPO-2D [6], based on the formulae given by Renau *et al.* [7], has been used (with 64-bit precision) to calculate the matrix elements A_{ij} and the capacitance C of the disc.

Figure 1 shows a log–log plot of the relative error $1 - C_N/C_{\text{exact}}$ versus the number N of segments, for m from 1 to 4, where C_{exact} is the exact value quoted above. At each value of m the results have been fitted by least-squares to the expression

$$C_N = C_{\text{exact}} + \sum_i a_i N^{-i}, \tag{3}$$

where the choice of indices i depends on the value of m. This should be regarded as an empirical fit, since it seems that there is at present no mathematical foundation for the assumption that the discretization error can be expressed as a polynomial in $1/N$ [1]. The best two least-squares fits are those for $m = 2$ and 4, for which it has been found that the appropriate values of i of the expansion terms are 2 and 3 for $m = 2$ (i.e., the term in $1/N$ is absent), and 3 and 4 for $m = 4$ (i.e., the terms in $1/N$ and $1/N^2$ are both absent). If C_{exact} is treated as an unknown and is deduced from these two fits, then it is given with a relative error of 4×10^{-8}. The fit for $m = 1$ is not quite as close and that for $m = 3$ is markedly poorer. If only the points for $N = 50$ and above are included, the relative error becomes 3×10^{-9} for $m = 2$ and 1×10^{-8} for $m = 4$. The choice $m = 2$ and extrapolation with $i = 2$ and 3 gives the smallest error for the capacitance of the disc, and also gives the closest fit to Eq. (3). We shall see below that this choice is also the most appropriate and the easiest to implement for the thin unit square, and so we recommend it for general use when thin plates are involved.

Another method of controlling the subdivision into segments is that of "adaptive segmentation," which is an option that exists in the CPO programs. In this method the segments are progressively subdivided in stages, the segments that carry the highest charges being given the largest number of subdivisions at each stage. This method is convenient for the general user, but it gives a final set of segments for which the variation in size is not a smooth function of position and is dependent on the total number N of segments. The relative error in a capacitance is then not a smooth function of N, and so we do not recommend this method when the highest accuracy is required and when at the same time distributions such as those given by Eq. (2) can be used.

The extrapolations with $m \geq 2$ are remarkably accurate, and are several orders of magnitude better than that with $m = 1$. In fact, distributions with $m = 2$ were first found empirically by Read *et al.* [8] to give increased accuracy in calculations of the focal properties of double cylinder lenses, and have since been used more generally [2, 7]. The variant of the BEM method used by Van Hoof [9] also implied the use of a distribution that is very close to the distribution that has $m = 2$, and gave a fast and accurate extrapolation for the capacitance of a disc.

The presence of the term in $1/N$ when $m = 1$ and its absence when $m > 1$ can be partially understood by considering the effects of the nonuniformity of the charge density on the surface of the disc, in particular the effect of the singularity in the charge density at the edge of the disc. For an edge that has an obtuse angle θ (e.g., 2π for a thin plate, $3\pi/2$ for the edge of a cube), the dependence of the charge density σ on the distance x from the edge is given by [5]

$$\sigma = \beta x^{-\alpha}, \tag{4}$$

where β is a constant and

$$\alpha = 1 - \pi/\theta. \tag{5}$$

The total charge on a segment at an edge, integrated over the width w of the segment, is therefore proportional to $\beta w^{-\alpha+1}$. For example, the charge density on a thin plate is $\beta x^{-1/2}$, and so integrating this over the segment at the edge of the plate gives the total charge $2\beta w^{1/2}$ for the segment. More generally, the integrated charge on a near-edge segment bounded by x_k and x_{k+1} is $2\beta(x_{k+1}^{1/2} - x_k^{1/2})$. In the distribution with $m = 2$ the distances x_k are proportional to k^2, which therefore causes all the segments near an edge to carry approximately the same charge.

The diagonal matrix elements A_{ii}, representing the self-potentials at the annular segments i due to their own charges, are in general significantly larger than the off-diagonal matrix elements, and so errors in them tend to dominate the error in a calculated capacitance or field. The expression for the diagonal elements is [7]

$$A_{ii} = (4\pi^2\varepsilon_0 r)^{-1}(\ln(16r/w) + 1), \tag{6}$$

if the charge density is uniform and if $w \ll r$, where r is the mean radius of the annular segment and w is its width. In fact, it is possible to remove the assumption of a uniform charge density and to integrate analytically over charge densities that have the form $x^{-1/2}$ for a thin plate. We find that the result for the end segment (which is given the label $i = 1$) of a flat disc is

$$A_{11}^{\text{non}-u} = (4\pi^2\varepsilon_0 r)^{-1}(\ln(16r/w) + 2 - 2^{1/2}\ln(2^{1/2} + 1)). \tag{7}$$

The difference between A_{11} and $A_{11}^{\text{non}-u}$, caused by the charge nonuniformity, is significant in practice, amounting for example to approximately 3% when $w/r = 0.01$. Furthermore, the difference depends only weakly on w (and hence only weakly on N).

To estimate the effect of this error on the calculated value of C, we start by supposing that A_{11} is the only element of A that is in error. Numerical simulations in which all the segments are taken to have approximately the same size (so that all the diagonal elements are approximately the same and the off-diagonal elements decrease approximately inversely with their distance from the diagonal) then show that the error in C is approximately proportional to $1/N$. The errors in the other diagonal elements A_{ii} are significantly smaller, as are those in the off-diagonal elements, and so the dependence on N of the error in C should not change significantly when these are taken into account. This therefore indicates that the presence of the $1/N$ term for the distribution that has $m = 1$ can be ascribed principally to the error in the evaluation of A_{11} in the present example. Numerical simulations of the distribution with $m = 2$ indicate that the relevant power of $1/N$ is approximately doubled. The removal of the term in $1/N$ is therefore clearly associated with the reduction in size of the edge segment and its immediate neighbours. When the distributions with $m = 3$ and 4 are used the edge and near-edge segments become relatively much smaller and the results discussed above show that the first term becomes that in $1/N^3$: at the same time the values of C_N become more accurate at small values of N, as can be seen in Fig. 1.

3. CAPACITANCES OF THE UNIT SQUARE AND CUBE

Exact determinations of the capacitances of the unit square and cube have long been regarded as two of the major unsolved problems of electrostatic theory [3, 4, 10, 12]. The most accurate values obtained so far for these capacitances appear to be those of Goto *et al.* [11], who used the BEM and claimed fractional inaccuracies of 3×10^{-6} and 8×10^{-7}, respectively. Goto *et al.* divided each edge of the square or cube into $2n$ equal parts (i.e., $m = 1$ in Eq. (2)), and the calculated capacitances C_n were found empirically to have the approximate form

$$C_n = C_\infty + \sum_i (a_i n^{-i} + b_i \ln(n) n^{-i}), \tag{8}$$

where the most appropriate choice of summation indices was found to be $i = 1$ and 2. The required extrapolation C_∞ was obtained for values of n typically in the region from 12 to 16, with a partially subjective discarding in the extrapolation process of some points that showed irregular behaviour.

We have investigated the n dependence of the calculated capacitance of the unit thin square when the distribution with $m = 2$ is applied. Equation (2) is used separately for the bounding values of the coordinates in the orthogonal x and y directions of the surface of the square, where R is replaced by half the length of a side of the square and N is replaced by n, the number of divisions of half a side. The resulting set of segments is shown in Fig. 2 for $n = 10$ (and then the total number of segments is $N = 400$). As mentioned above, this method of subdivision should cause all the segments near an edge to carry approximately the same charge. The nonlinearity of the charge density at the corners of the square is even stronger than at the edges (our computations show that the exponent α in Eq. (4) is 2/3), but the segments in this region are overcompensated in the sense that their areas are proportional to $1/n^4$.

The requirement that the segments in the vicinity of an edge should all carry approximately the same charge has also been imposed for the subdivision of the faces of the unit cube, and is achieved by using the nonintegral power $m = 3/2$ in Eq. (2). For both the square and the cube the results are well fitted by the expression

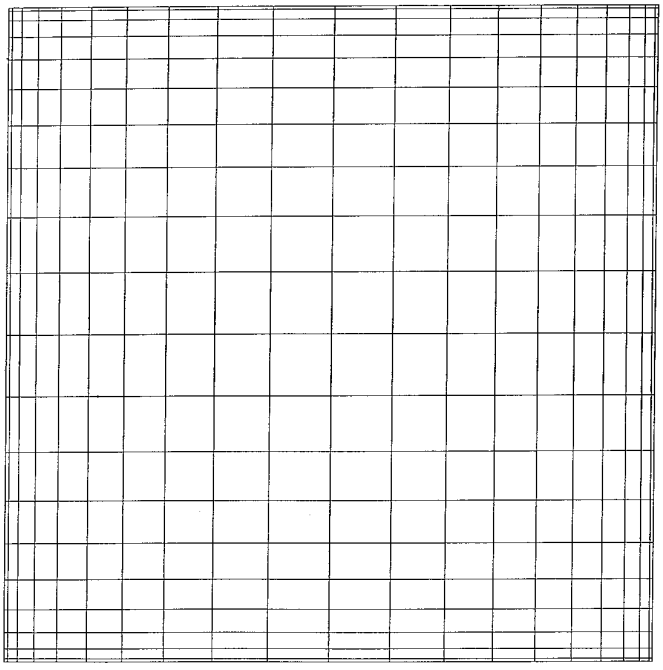

FIG. 2. Division of a square into segments, using the exponent $m = 2$ in Eq. (2) (see text) in both the horizontal and vertical directions.

$$C_n = C_\infty + \sum_i a_i n^{-i}, \tag{9}$$

where the summation is over $i = 2$, 3, and 4. We see therefore that the term in $1/n$ has been eliminated by this strategy and that the terms in $\ln(n)$ are also not needed. Note that the total number N of segments is proportional to n^2, and so the leading term is proportional to $1/N$ (as opposed to a leading term of $1/N^{1/2}$ in the method of Goto *et al.*). It has not been possible, for the square and cube, to carry out the analogous integration that led to Eq. (7), to find the change in the self-potential matrix element A_{ii} when the charge density is nonuniform, but the present results indicate that this change is again significant and that it depends only weakly on n. The values of a_i/C_∞ for the unit square are (to 3 significant figures) -0.198, 0.0693, and -0.00405, and for the unit cube they are -0.0462, 0.0152, and -0.00681, in both cases for $i = 2$, 3, and 4 respectively.

The capacitance of the square has also been computed using the distribution with $m = 3$, but the rectangular segments at the edges then have a large ratio of their longest to shortest side, and so it is necessary to subdivide them along their length. The fits to Eq. (9) are less close, but are consistent with the results obtained using the distribution with $m = 2$. Expansions of the type given by Eq. (8) have also been tried: the resulting fits are poorer but the deduced capacitances are still consistent with the more accurate values. Similarly, the capacitance of the cube has been computed using the distributions with $m = 2$ and 3, and also Eq. (8) has been used in addition to Eq. (9) to fit the results, but the fits are not as close as those obtained with the nonintegral exponent $m = 3/2$ and with Eq. (9). The strategy that has often been followed empirically in the past [2, 6–9], that of adjusting the sizes of the segments so that those near an edge all carry approximately the same charge, is therefore found to be the best one for the present problem.

The values obtained (using the CPO-3D program [6], in 64-bit precision) for the capacitances by this extrapolation technique are given in Table I. The errors are conservative values based on least-squares fits of Eq. (9) using a set of different ranges of n. The maximum values of n that have been used are 29 for the square (giving a total of 3364 segments for the complete square, after reflection in two planes of symmetry) and 17 for the cube (corresponding to a total of 6936 segments for all 6 faces of the cube), and at these maximum values the computing times are of the order of 30 min, using a 66-MHz 486 PC. The capacitances are given in units of $4\pi\varepsilon_0$, the value of which is 111.265006 pF/m. For a square or cube of side 1 m the capacitances obtained in the present study are therefore 40.81060 ± 0.00001 pF and 73.51040 ± 0.00007 pF respectively. The present result for the cube precludes the conjectured [12, 13] exact value of 0.6594 ... (in units of $4\pi\varepsilon_0$).

The present results have estimated relative errors of 3×10^{-7} and 3×10^{-6} for the square and cube respectively, and differ from the results of Goto *et al.* by approximately 5×10^{-6} and 6×10^{-6} respectively. The improvement in accuracy is therefore approximately an order of magnitude. Interestingly, the value obtained by Maxwell [3, 4] for the unit square, using primitive numerical evaluations, was 0.3638, which is in error by only 0.8%.

Finally, it should be noted that when the object that is under study does not have any significant edges (i.e., when the exponent α in Eq. (4) is nearly zero), as for a sphere, the expansion of C_N automatically has a first expansion term in $1/N^2$, even when all the segments have approximately the same dimensions, and so there is essentially no limit to the accuracy obtainable with the boundary element method (apart from machine rounding errors).

TABLE I

Capacitances in Units of $4\pi\varepsilon_0$ of the Unit Square and Cube

Shape	Goto *et al.* [11]	Present results
Unit square	0.3667892 ±0.0000011	0.3667874 ±0.0000001
Unit cube	0.6606747 ±0.0000005	0.6606785 ±0.0000006

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