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## Method of moments and the use of multipole expansion

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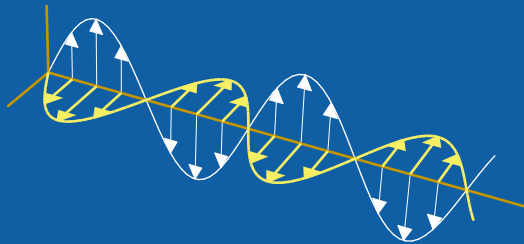
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**Abstract**

In electromagnetic boundary value problems integral equations involving the free space Green's function for the Helmholtz equation often occur. Using the method of moments to numerically solve such an equation a matrix equation is obtained. The entries of the matrix are given as multidimensional integrals which in general have to be calculated numerically. This paper presents an efficient method to approximate the main part of these integrals. The free space Green's function is expanded in scalar spherical wave functions. The translation properties of these wave functions then imply that the matrix elements can be expressed as a series of multipole moments. The method is illustrated by an implementation in the static case - the computation of the capacitance of a square plate. Basis functions with the correct edge and corner behaviour are used. The calculations of the multipole moments are done analytically. Numerical results using the point-matching and Galerkin's method are presented.

## 1. Introduction

Electromagnetic boundary value problems are often formulated as integral equations containing the free space Green's function for the Helmholtz equation. The unknown function usually represents some source distribution to be determined. A method frequently used to solve these integral equations numerically is the method of moments (MoM) [1]. Basically, the method of moments is a projection method, where the original integral equation is replaced by a finite dimensional matrix equation, which entries are multidimensional integrals. In general these matrix elements cannot be calculated analytically and numerical integration or various approximations are adopted. Galerkin's method, which is favoured by many authors, implies that the matrix is symmetric. This symmetry property is, however, usually lost when approximations are introduced in the calculations of the matrix elements. Since high numerical performance is necessary in modern computations, the development of approximation schemes that preserves this symmetry is valuable.

In this paper an approximation method using multipole expansion is presented. The three-dimensional case is analysed and the free space Green's function for the Helmholtz equation is expanded in terms of the scalar spherical wave functions. Using subsectional basis and weighting functions and taking advantage of the translation properties of the scalar spherical wave functions the main part of the matrix elements can be expressed as a series of multipole moments. One of the main advantage of the multipole expansion is that the bulk of the entries of the matrix can be approximated by only a few terms in this expansion, leaving a few diagonal terms left for more accurate considerations. Moreover, this approximation method also preserves the symmetry of the matrix when Galerkin's method is used. Special attention is paid to the static limit and the numerical performance of the approximation is illustrated by the computation of the capacitance of a square plate. Basis functions with the correct edge and corner behaviour are used. The point-matching method as well as Galerkin's method are applied. It is in this context relevant to point out that the approach presented in this paper differs from recent formulations utilizing multipole expansions [2] which do not use the method of moments.

The plan of the paper is as follows. Section 2 contains an overview of the technique used in the MoM. The approximation method using the multipole expansion is derived in Section 3. In Section 4 the method is applied to calculate the capacitance of a square plate. Diagrams illustrating the efficiency of the approximation and the enhanced convergence due to the singular basis functions are presented in Section 5. Some conclusions are given in Section 6. In Appendix A the relevant formulas concerning the translation properties of the scalar spherical wave functions are summarized. In Appendix B the

static limit of the translation properties is derived. Some technical details are presented in Appendix C.

## 2. Method of moments

The method of moments is an established technique to numerically solve linear operator equations. It is frequently applied to integral equations of the first and second kind. The MoM, which is a projection method, approximate the solution to the original infinite dimensional problem by a finite dimensional solution. Projection methods in general, and MoM in particular, are well-established methods, but for the sake of completeness and to introduce our notations a short overview of the concept of the MoM is given. Only the formal steps of the MoM are presented here. The readers interested in the more rigourous mathematical aspects of the theory, e.g. convergence and completeness properties of basis functions, are referred to, e.g., [3].

The linear operator equation is written as

$$L(f) = g \tag{1}$$

where $L$ denotes the linear operator, $g$ is the known function and $f$ is the function to be found. The first step is to expand $f$ in terms of a set of known basis functions $f_p$ in the domain of $L$, with unknown coefficients $\alpha_p$.

$$f \approx f_Q = \sum_{p=1}^{Q} \alpha_p f_p \tag{2}$$

As $L$ is linear we have

$$L(f_Q) = \sum_{p=1}^{Q} \alpha_p L(f_p) \approx g \tag{3}$$

Now form the residual $R_Q$

$$R_Q = L(f_Q) - g \tag{4}$$

Finally choose a set of weighting functions, $w_q$, in the range of $L$ and take the inner product of (4)

$$<R_Q, w_q> = 0 \qquad q = 1, 2, \dots Q \tag{5}$$

The inner product is usually defined as

$$<a, b> = \int_D a(z)b(z) \, dz \tag{6}$$

where $D$ denotes the domain of $a$ and $b$.

The relation (5) can be written as

$$\sum_{p=1}^{Q} \alpha_p <L(f_p), w_q> = <g, w_q> \qquad q = 1, 2, \dots Q \tag{7}$$

The coefficients $\alpha_p$ are obtained by solving this matrix equation.

Certain choices of the weighting functions $w_q$ correspond to methods with their own names, e.g.:

$$w_q(z) = \delta(z-z_q)$$  The point-matching method or Collocation method

$$w_q(z) = f_q(z)$$  Galerkin's method

$$w_q(z) = L(f_q)(z)$$  The method of least squares

The point-matching method is widely used due to its simplicity. In Galerkin's method the calculations of the matrix elements generally become very time consuming if no approximations are made. The method of least squares is probably the most reliable, but also the most complex of the three methods.

The choice of the basis functions does also to a high degree affect the calculation time of the matrix elements. The method of moments is often associated with the use of subsectional basis functions. This involves the use of basis functions $f_p$ each of which only differs from zero over subsections of the domain of $f$. Usually polynomials of low degree are used as basis functions over these subsections.

The choice of basis functions does, however, also affect the achievable accuracy of the approximation of $f$ for a certain truncation $Q$. It is often possible to analytically determine the behaviour of $f$ at, e.g., the boundary of the domain. By choosing basis functions with appropriate behaviour higher accuracy can be obtained. More complex basis functions will, however, generally lead to an increase of the calculation time of the matrix elements. It is obvious that it is essential to find efficient approximation methods for calculating the matrix elements.

## 3.  Multipole expansion

The three-dimensional case is considered in this paper. Space vectors are denoted bold face, and $R_p$ denotes the position of a fixed point $p$ in space with respect to a general origin. $R_{pq}$ denotes the vector from point $p$ to point $q$, i.e. $R_{pq}=R_q-R_p$. A lower case vector without index refers to a general origin, while those with index refer to local origins, cf. Fig. 1. Whenever possible, we distinguish between source and field points, by a prime on the vectors referring to a source point.
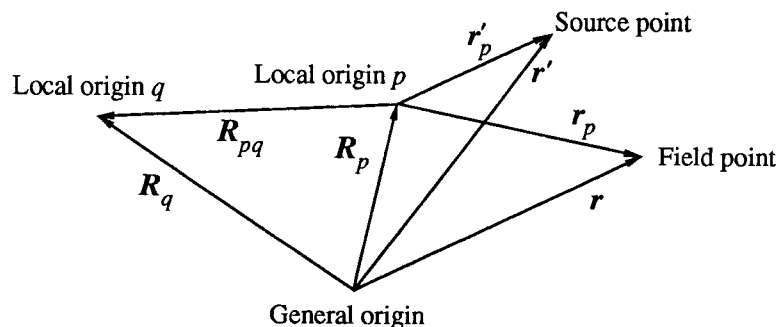


Fig. 1. Space vector notations

When working with electromagnetic scattering and electrostatic problems in three-dimensional space the following integral operator frequently occurs

$$L(f) = \int_{V'} f(r') \; G(r,r') \; dv' \tag{8}$$

where $r'$ is the integration variable and $G(r,r')$ is the free space Green's function.
In the time harmonic case, $G(r,r')$ is given by

$$G(r,r') = \frac{e^{ik|r-r'|}}{4\pi \; |r-r'|} \tag{9}$$

where $k$ is the wave number and the time factor $e^{-i\omega t}$ is suppressed. The electrostatic case is obtained as the limit $k \to 0$.
Applying the method of moments we get matrix elements of the following kind

$$<L(f_p),w_q> = \int_{V} \int_{V'} f_p(r') \; G(r,r') \; dv' \; w_q(r) \; dv \tag{10}$$

Using point-matching, one obtains

$$<L(f_p),\delta_q> = \int_{V'} f_p(r') \; G(R_q,r') \; dv' \tag{11}$$

where $\delta_q = \delta(r-R_q)$. The delta function $\delta_q$ is assumed to have support near the local origin $R_q$.
In cases where $r > r'$, $G(r,r')$ can be expanded [4] in the scalar spherical wave functions $\psi^i_{\sigma ml}$ and $\psi^e_{\sigma ml}$

$$G(r,r') = ik \sum_n \psi^i_n(r') \; \psi^e_n(r) \tag{12}$$

where the summation over $n$ denotes a triple sum over $l,m$ and $\sigma$.
The scalar spherical wave functions are defined as

$$\psi^i_{\sigma ml}(r) = j_l(kr) \; Y_{\sigma ml}(\hat{r}) \tag{13}$$

$$\psi^e_{\sigma ml}(r) = h^{(1)}_l(kr) \; Y_{\sigma ml}(\hat{r}) \tag{14}$$

where $j_l$ is the spherical Bessel function, $h^{(1)}_l$ the spherical Hankel function of the first kind and $Y_{\sigma ml}$ is the spherical harmonic defined by

$$Y_{\sigma ml} = \left( \frac{\varepsilon_m}{2\pi} \frac{2l+1}{2} \frac{(l-m)!}{(l+m)!} \right)^{1/2} P^m_l(\cos\theta) \begin{pmatrix} \cos m\phi \\ \sin m\phi \end{pmatrix} \tag{15}$$

Here $P^m_l$ is the Associated Legendre function and $\varepsilon_m = 2 - \delta_{m0}$, $l = 0,1,...,$ $m = 0,...l$ and $\sigma = e,o$ (even,odd). We employ the definitions in Ref. [5] for the Bessel, Hankel and Associated Legendre functions.
Now let $f_p(r') = 0$ outside the subsection $V'_p$ and introduce a circumscribed sphere (radius $r'_{pmax}$) to the subsection. Let the centre of the sphere define the origin of a local spherical coordinate system $K_p$, cf. Fig. 2.
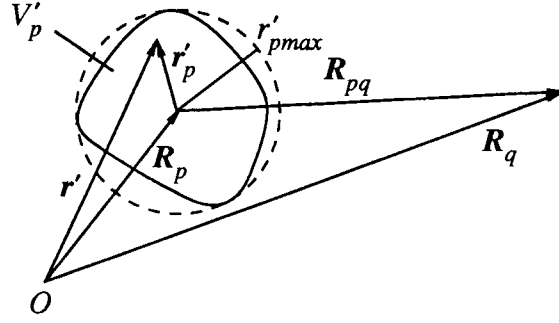
Fig. 2. The subsection $V'_p$ and a circumscribed sphere

At points outside the sphere, i.e. when $R_{pq} > r'_{pmax}$, Eq.(11) can be written as

$$<L(f_p),\delta_q> = ik \sum_n q_n(f_p) \, \psi_n^e(R_{pq}) \tag{16}$$

where

$$q_n(f_p) = \int_{V'_p} f_p(r') \, \psi_n^i(r'_p) \, dv' \tag{17}$$

$q_n(f_p)$ expresses the multipole moments associated with the basis function $f_p$. When these moments have been calculated all those matrix elements that correspond to $R_{pq} > r'_{pmax}$ are easily obtained.

The more general expression for the matrix elements Eq.(10) may, under the same conditions as above, be rewritten as

$$<L(f_p),w_q> = \int_V \int_{V'_p} f_p(r') \, G(r_p,r'_p) \, dv' \, w_q(r) \, dv =$$

$$= ik \sum_n \int_{V'_p} f_p(r') \, \psi_n^i(r'_p) \, dv' \int_V w_q(r) \psi_n^e(r_p) \, dv \tag{18}$$

where the notations are defined in Fig. 3. The volume $V$ is here any volume outside the circumscribing sphere of $V'_p$.
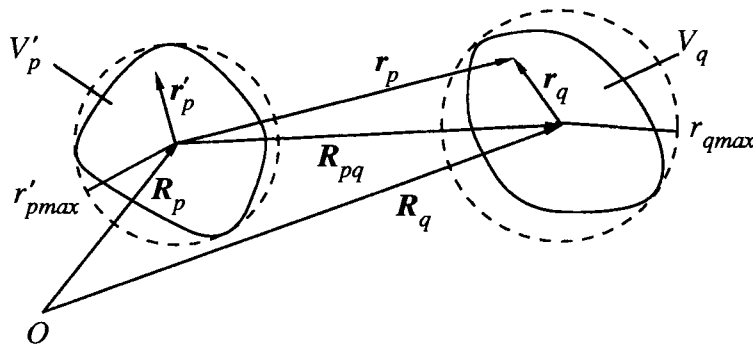


Fig. 3. The two interacting subsections $V'_p$ and $V_q$

Now, let the weighting function $w_q$ be zero outside the subsection $V_q$. Introduce a circumscribed sphere (radius $r_{qmax}$) and define a local coordinate system $K_q$ at the origin

of the sphere. Furthermore, let the orientation of the coordinate axes of the two systems $K_p$ and $K_q$ coincide. If the distance between the two local origins is greater than the radius of the sphere i.e., $R_{pq} > r_{qmax}$, then the wave function $\psi_n^e(r_p)$ can be expressed in the new coordinates as [4]

$$\psi_n^e(r_p) = \sum_{n'} P_{nn'}(R_{pq})\ \psi_{n'}^i(r_q),$$ (19)

for all $r_q \in V_q$.

The matrix $P_{nn'}$ is given in Appendix A. Inserting Eq.(19) into Eq.(18) results in

$$<L(f_p),w_q> = ik \sum_{nn'} P_{nn'}(R_{pq})\ q_n(f_p)\ q_{n'}(w_q)$$ (20)

provided summation and integration can be changed. This is allowed when $R_{pq} > r'_{pmax} + r_{qmax}$, due to uniform convergence of the series. The functional $q_n(f_p)$ is given by Eq.(17) and $q_n(w_q)$ is similarly defined as

$$q_n(w_q) = \int_{V_q} w_q(r)\ \psi_n^i(r_q)\mathrm{d}v$$ (21)

In the numerical implementation the summations have to be truncated. When $n$ and $n'$ are truncated equally, the reciprocity of Eq.(10) is preserved in the approximation. Hence using Galerkin's method, with $q_n(w_q) = q_n(f_q)$ , the matrix of Eq.(7) will be symmetric. Therefore, just half of the non-diagonal matrix elements have to be calculated and numerical routines designed to symmetric matrices can be used when solving the equation.

## 4.  Capacitance of a square plate

The exact charge distribution and capacitance of a charged infinitely thin, conducting, flat square plate in unbounded space is not known. Several authors, e.g. [1], [6] and [7], have used moment methods to obtain numeric solutions. Methods involving simple basis functions, such as pulse or roof-top functions which do not have the correct asymptotic behaviour at the edges and corners, will converge [8], but very slowly. In the analogous two-dimensional case, it is known from the literature [9], [10] that the correct edge behaviour in the basis functions will improve the convergence. The corner singularity in the three-dimensional case has been calculated in Refs. [11]-[14], using different analytical methods combined with numerical algorithms. In the approximation method described in Section 3, it is possible to introduce the edge and corner singularities in the basis functions without any major difficulty.

The electrostatic potential $V(r)$ caused by a finite charged conductor in homogeneous unbounded space is given by ( if $r\ V(r) \to$ constant as $r \to \infty$ )

$$V(r) = \frac{1}{4\pi\varepsilon} \int_{S'} \sigma(r') \frac{1}{|r-r'|}\ \mathrm{d}S'$$ (22)

where $S'$ is the surface of the conductor, $\sigma(r')$ is the surface charge density and $\varepsilon$ is the permittivity of space outside S'. If we suppose that the constant potential at the plate,$V_0$, is known, we obtain a linear integral equation of the first kind given by Eq.(8). The static

limit as $k \to 0$ of the analysis presented in Section 3 is described in Appendix B. The capacitance $C$ of the conductor is defined as

$$C = \frac{1}{V_0} \int_{S'} \sigma(r') \, dS'$$

(23)

Divide the plate into Q equally sized square subsections. Number the subsections from 1 to Q. Denote the length of the side of each subsection $p$ by $2\Delta$. Define a basis function $f_p$ on each subsection $p$ such that $f_p = 0$ outside the subsection. The approximation $\sigma_Q$ of $\sigma$ can then be written

$$\sigma_Q = \sum_{p=1}^{Q} \alpha_p f_p$$

(24)

We have used three different types of basis functions depending on the position of the plate. $f_p^C$ is used on the subsections at the corners, $f_p^E$ on the subsections at the edges and $f_p^I$ on the interior subsections. On each subsection the basis functions are expressed in local Cartesian coordinates with the origin in the centre of the subsection and with the x- and y-axes parallel with the edges of the subsection. The basis functions are defined as follows:

$$f_p^I = 1$$

(25)

$$f_p^E = \frac{1}{\sqrt{1-x/\Delta}}$$

(26)

$$f_p^C = \frac{(\sqrt{2})^{\lambda-2}}{\left((1-x/\Delta)^2+(1-y/\Delta)^2\right)^{\lambda/2}} \left( \sqrt{\frac{1-y/\Delta}{1-x/\Delta}} + \sqrt{\frac{1-x/\Delta}{1-y/\Delta}} \right)$$

(27)

where $\lambda=0.70$ [11]-[14]. The local coordinate system for each subsection has to be orientated with respect to the edges and corners, so that the correct singular behaviour is obtained.

As shown in Appendix C the static multipole moments of these basis functions can be analytically calculated.

The capacitance was calculated using the point-matching method and the method of Galerkin. In the next section the numerical results are presented.

## 5. Numerical results

In the point-matching method, the matrix elements corresponding to the interior basis functions, i.e. the potential from a constant charge distribution, can be calculated analytically. This was used to find the error in the multipole approximation technique. In Fig. 4 and Fig. 5 the relative error as a function of the distance is plotted using different truncations. $L$ denotes the maximum value of the summation index $l$, cf. Eq.(B3). The radius of convergence of the multipole expansion is $\sqrt{2}\,\Delta$, see Section 3 and [4]. Figures 4 and 5 clearly confirm this property, and the numerical results do well agree with the theory.

The Galerkin's case is illustrated in Figs. 6 and 7. The reference values were in this case obtained by numerical integration. The indices $l$ and $l'$, cf. Eq.(B5), are both truncated to $L$. Although convergence can not be expected when the distance is less than $2 \sqrt{2} \Delta$, the accuracy in the x-direction is reasonable even for lower values of $d/\Delta$. Other approximation schemes to simplify the computations in projection methods have been suggested in the literature [15]. If the analogous technique is adopted in our static case, we obtain the shadowed curves in Figs. 6 and 7. The outer integral of Eq.(10) is calculated by approximating the inner integral by its value at the centre of the subsection. It is clearly shown that the approximation scheme suggested in this paper provides a great improvement in accuracy.

The capacitance of the square plate was calculated using the point-matching method and the method of Galerkin. When the point-matching method was applied, collocation points at the centre of each subsection were used. In both cases, all the non-diagonal matrix elements were calculated using the multipole approximation. Hence, in the Galerkin case, the convergence rules were violated when computing matrix elements corresponding to adjacent subsections. This was noticed as a slightly variation of the obtained capacitance dependent on the chosen truncation. As comparison the capacitance was also calculated using constant basis functions in all subsections. The point-matching case can be found in [1]. The results are shown in Fig. 8. The convergence is, as seen, greatly enhanced when basis functions having the correct the edge and corner singularities are used.
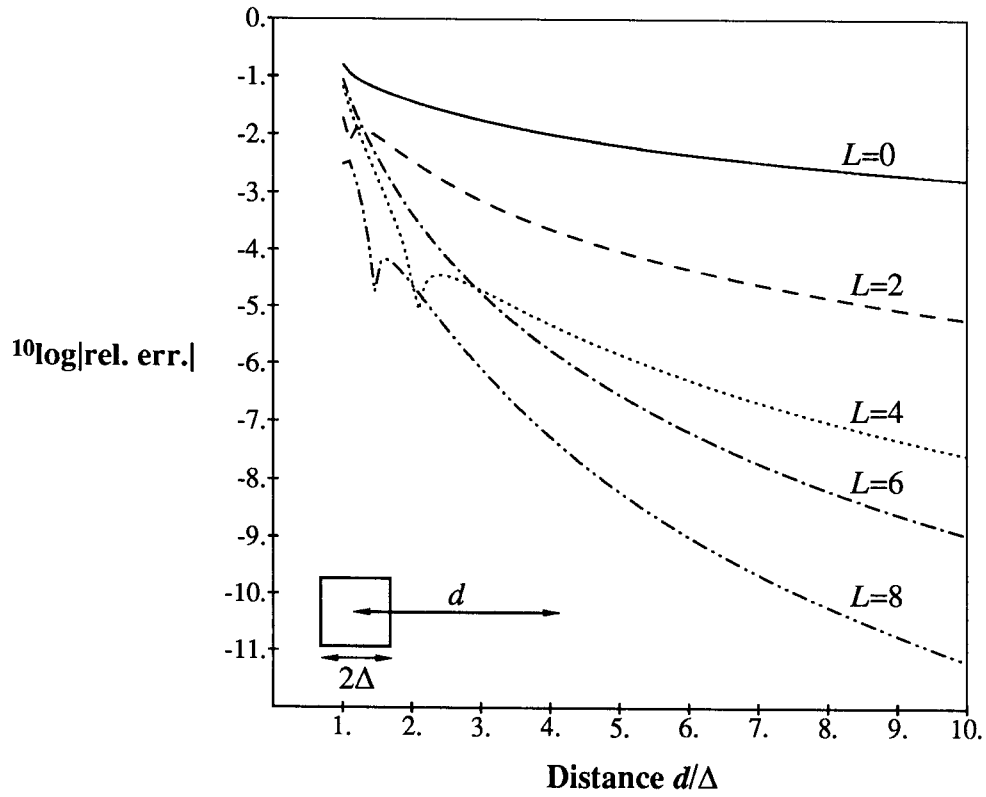
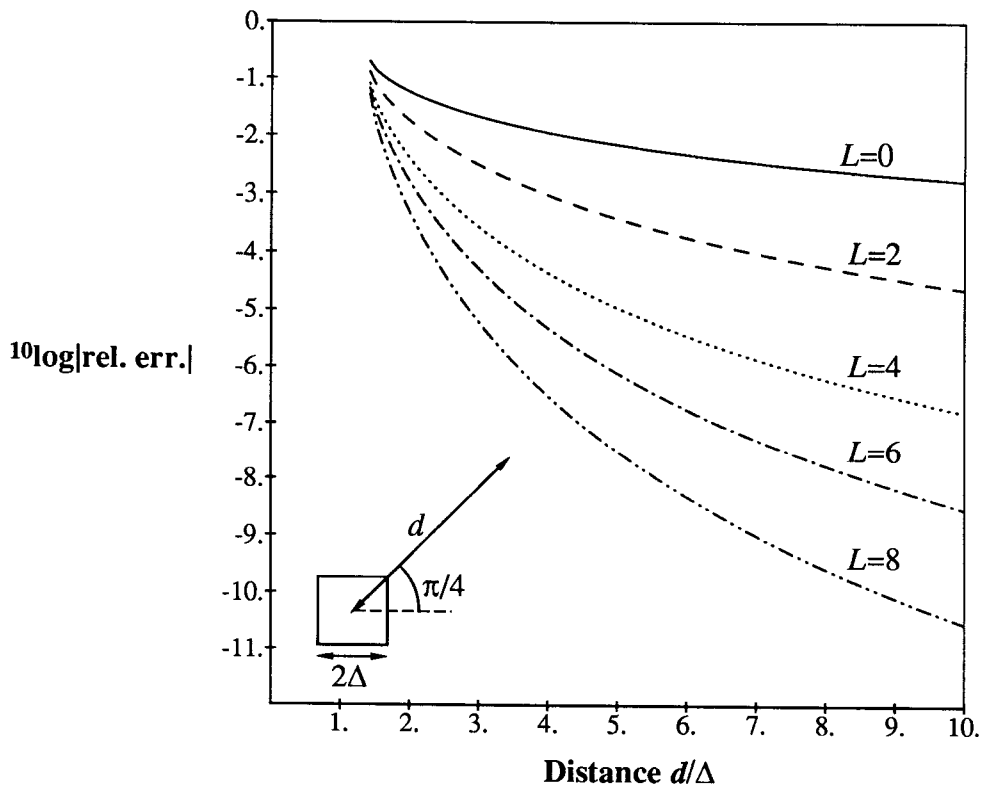Fig. 4. Point-matching, the relative error in the x-direction



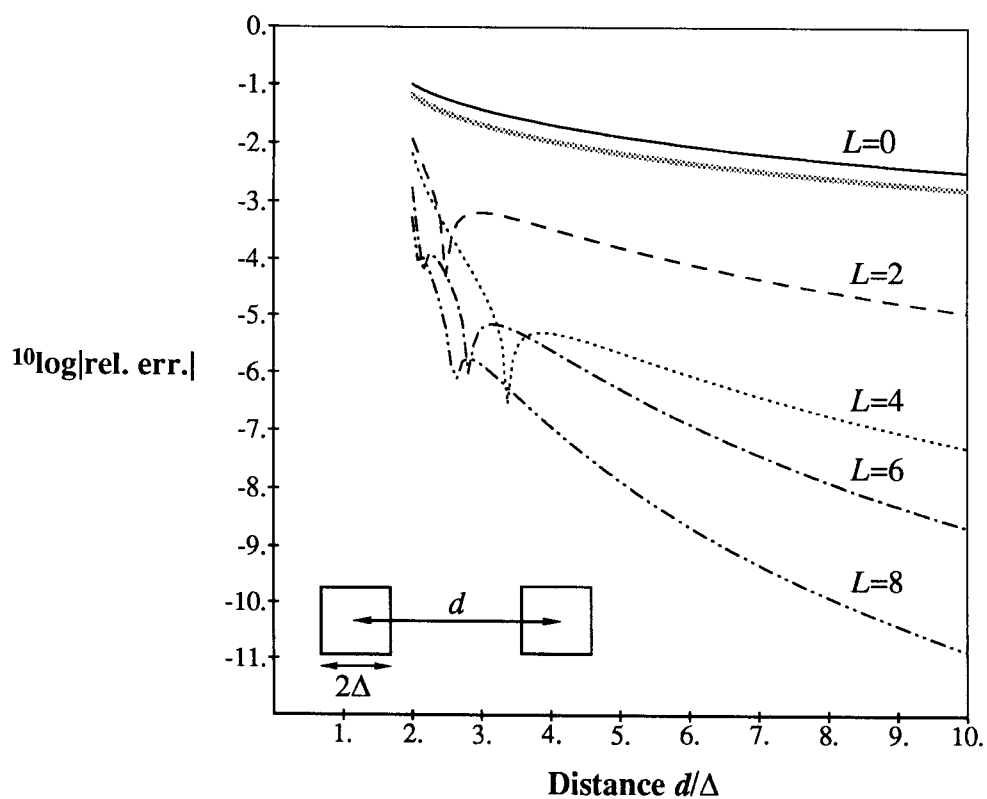Fig. 5. Point-matching, the relative error in the xy-direction

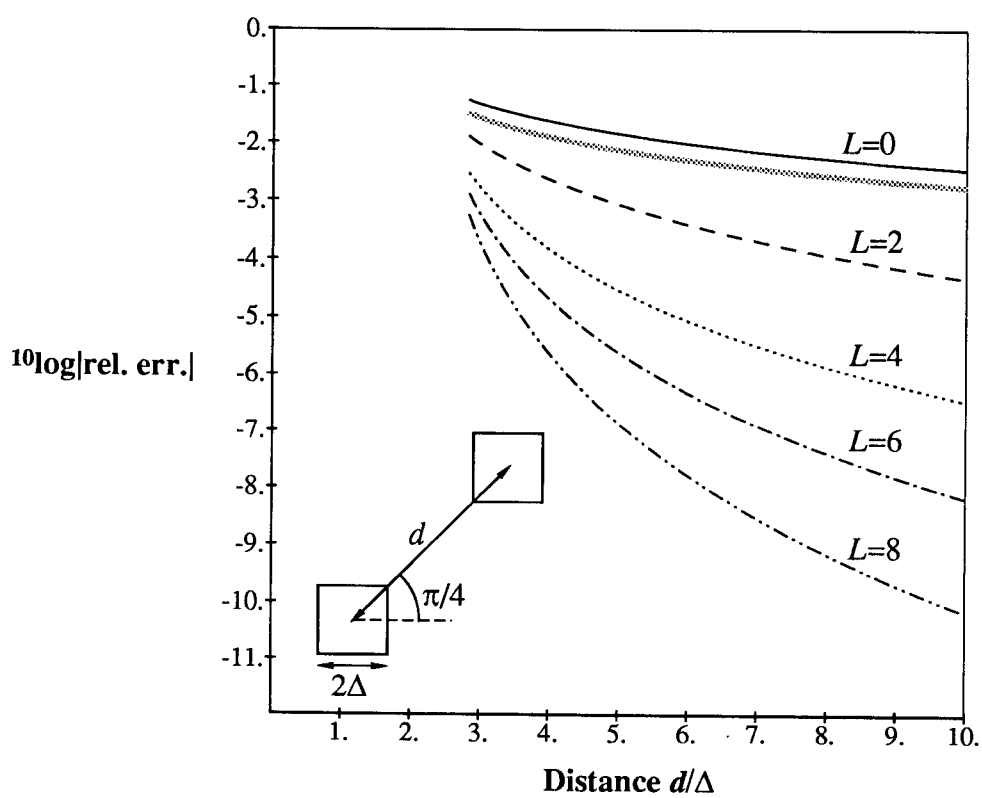Fig. 6. Galerkin's method, the relative error in the x-direction



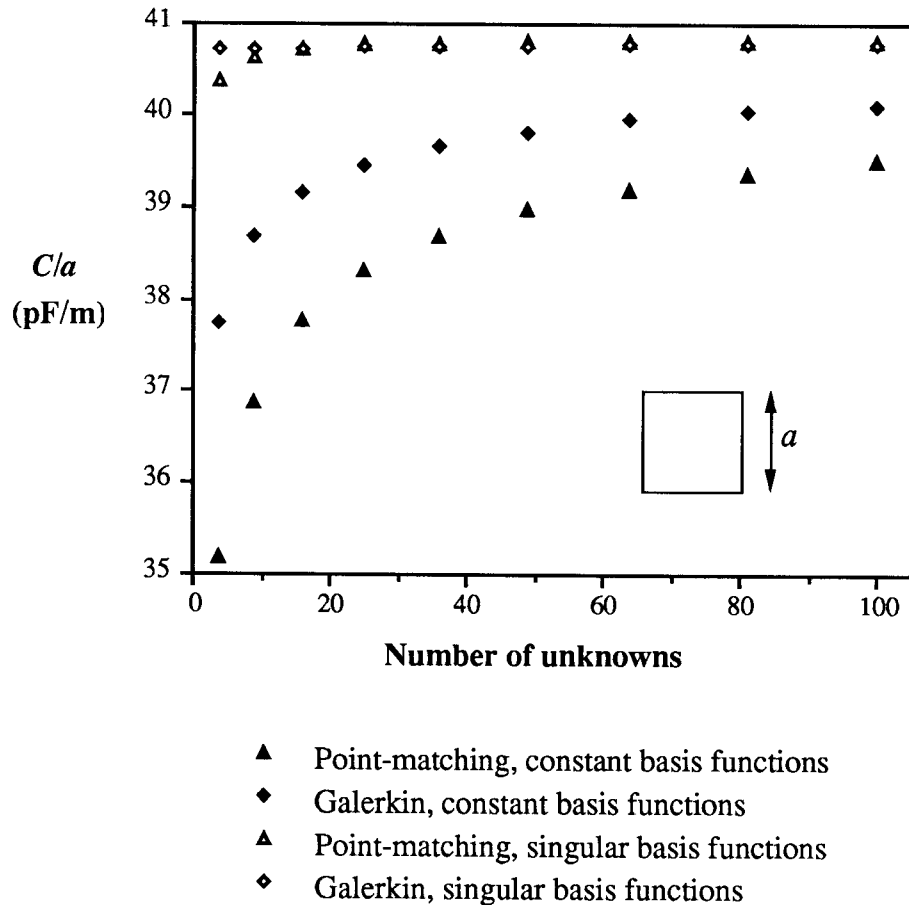Fig. 7. Galerkin's method, the relative error in the xy-direction

Fig. 8. The capacitance of a square plate with side of length $a$

# 6. Summary and conclusion

Electromagnetic boundary value problem can be solved numerically by the method of moments. The appropriate integral equation is then replaced by a matrix equation. In this paper a method to compute the main part of the matrix elements as a series of multipole moments has been presented. The technique is applicable to integral equations in which the kernel consists of the free space Green's function of the Helmholtz equation. The three-dimensional case was considered. It can be noticed that using cylindrical wave functions, rather than the spherical ones used in this paper, the method may be adapted to two-dimensional space in a straightforward manner. The expansion of the two-dimensional Green's function in cylindrical wave functions as well as the translation properties of these wave functions are well known [4].

The method was applied to a canonical static problem - the calculation of the capacitance of a square plate. The accuracy of the approximations of the matrix elements has been illustrated. The method simplifies the use of complicated basis and weighting functions. Hence, basis functions with the correct edge and corner behaviour could be chosen and greatly enhanced convergence was obtained using the point-matching method as well as the method of Galerkin. When Galerkin's method was used only half of the non-diagonal matrix elements had to be computed as the approximation preserves the symmetry of the matrix.

The presented approximation method may obviously be applied to a wide range of static problems. Without loosing the simple structure, more advanced basis functions, such as

bilinear or Hermite bicubic functions, may be used. Other polygonial shapes of subsections, e.g. triangles, can be introduced. Another convenient property with the approximation method suggested in this paper is the calculation of the external field. The external field is obtained by simply adding all contributions from the multipoles. The method is, therefore, attractive from several points of view. The calculations of the external field is, however, not pursued in this paper, but will be addressed in a subsequent paper on the dynamic case. Work is in progress on this case and will be presented elsewhere.

## Appendix A

The transformation properties of the scalar wave functions can be found in Ref. [4]. This appendix summarizes important formulas concerning the translation properties of the scalar spherical wave functions.

Denote by $K_0$ and $K_1$ two spherical coordinate systems with different origins but with parallel axes, cf. Fig. A1. Let the origin of $K_1$ have the coordinates $(R,\eta,\varphi)$ (space vector $R$) in $K_0$. Let an arbitrary point in space be described by the space vectors $r_0$ and $r_1$ with reference to $K_0$ and $K_1$, respectively.
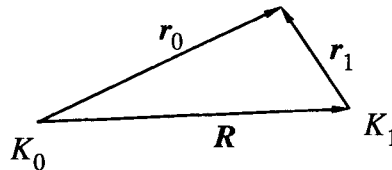


Fig. A1

We then have

$$\psi_n^e(r_0) = \sum_{n'} P_{nn'}(R)\ \psi_{n'}^i(r_1) \qquad\qquad R > r_1 \tag{A1}$$

$$\psi_n^i(r_0) = \sum_{n'} R_{nn'}(R)\ \psi_{n'}^i(r_1) \qquad\qquad (\text{ valid everywhere }) \tag{A2}$$

The matrices $R_{nn'}$ and $P_{nn'}$ are given by

$$R_{nn'}(R) = S_{nn'}(R;j_\lambda) \tag{A3}$$

$$P_{nn'}(R) = S_{nn'}(R;h_\lambda^{(1)}) \tag{A4}$$

$S_{nn'}(R;z_\lambda)$ may be written

$$S_{\sigma ml,\sigma m'l'}(R;z_\lambda) = \quad (-1)^{m'} B_{ml,m'l'}(R,\eta;z_\lambda)\ \cos(m-m')\varphi$$

$$+ (-1)^\sigma B_{ml,-m'l'}(R,\eta;z_\lambda)\ \cos(m+m')\varphi \tag{A5}$$

$$S_{\sigma ml,\sigma' m'l'}(R;z_\lambda) = \quad (-1)^{m'+\sigma'} B_{ml,m'l'}(R,\eta;z_\lambda)\ \sin(m-m')\varphi$$

$$+ B_{ml,-m'l'}(R,\eta;z_\lambda)\ \sin(m+m')\varphi \qquad\qquad \sigma \ne \sigma' \tag{A6}$$

where

$$(-1)^\sigma = \begin{cases} 1 & \sigma = e \\ -1 & \sigma = o \end{cases}$$

and

$$B_{ml,m'l'}(R,\eta;z_\lambda) = (-1)^{m+m'} \left(\frac{\varepsilon_m \varepsilon_{m'}}{4}\right)^{1/2} \sum_{\lambda=|l-l'|}^{l+l'} (-1)^{(l'-l+\lambda)/2} (2\lambda+1)$$

$$\times \left(\frac{(2l+1)(2l'+1)(\lambda-(m-m'))!}{(\lambda+(m-m'))!}\right)^{1/2} \begin{pmatrix} l & l' & \lambda \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l & l' & \lambda \\ m & -m' & m'-m \end{pmatrix}$$

$$\times z_\lambda(k R) P_\lambda^{m-m'}(\cos\eta) \tag{A7}$$

The definition of the Wigner 3-j symbol $\begin{pmatrix} \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \end{pmatrix}$ can be found in, e.g. [16].

## Appendix B

In this appendix the static limit, $k \to 0$, of the results reviewed in Appendix A is presented. More specifically, the translation properties of the static, scalar spherical wave functions are given. In this context it should be noted that these properties can be obtained by other means [17]-[20]. It is, however, advantageous for future work on the dynamic case to pursuit the $k \to 0$ limit approach in this paper.

When $kr \ll 1$ the spherical Bessel and Hankel functions have the following asymptotic properties [5]

$$j_l(kr) \to \frac{(kr)^l}{(2l+1)!!} \tag{B1}$$

$$h_l^{(1)}(kr) \to -i\frac{(2l-1)!!}{(kr)^{l+1}} \tag{B2}$$

Using the point-matching method, the matrix elements are given by Eq.(16). Hence, when $kr \ll 1$ we have

$$<L(f_p),\delta_q> \to k\sum_n \int_{V_p'} f_p(r')\frac{(kr_p')^l}{(2l+1)!!} Y_{\sigma ml}(\hat{r}_p')dv' \; \frac{(2l-1)!!}{(kR_{pq})^{l+1}}Y_{\sigma ml}(\hat{R}_{pq})$$

In the limit $k \to 0$ the electrostatic matrix elements are obtained as

$$<L(f_p),\delta_q> = \sum_n q_n^0(f_p) \; (2l-1)!! \; \frac{Y_{\sigma ml}(\hat{R}_{pq})}{R_{pq}^{l+1}} \tag{B3}$$

where

$$q_n^0(f_p) = \frac{1}{(2l+1)!!} \int_{V_p'} f_p(r') \; r_p'^l \; Y_{\sigma ml}(\hat{r}_p')dv' \tag{B4}$$

Inserting Eq.(B1) into the more general expression for the matrix elements, Eq.(20), one obtains in the same way

$$<L(f_p),w_q> = \sum_{nn'} P_{nn'}^0(R_{pq}) \; q_n^0(f_p) \; q_{n'}^0(w_q) \tag{B5}$$

where the matrix $P_{nn'}^0$ is given by

$$P_{nn'}^0 = \lim_{k \to 0} ik^{l+l'+1} P_{nn'} \tag{B6}$$

From Eqs.(A4) - (A7) we get

$$P_{nn'}^0(R) = S_{nn'}(R; \lim_{k \to 0} ik^{l+l'+1} h_\lambda^{(1)}) \tag{B7}$$

Taking the limit of Eq.(A7) using Eq.(B2) results in

$$B_{ml,m'l'}(R,\eta; \lim_{k\to 0} ik^{l+l'+1}h_\lambda^{(1)}) = (-1)^{m+m'+l'}\left(\frac{\varepsilon_m\varepsilon_{m'}}{4}\right)^{1/2}(2l+2l'+1)!!$$

$$\times \left(\frac{(2l+1)(2l'+1)(l+l'-(m-m'))!}{(l+l'+(m-m'))!}\right)^{1/2}\begin{pmatrix} l & l' & l+l' \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} l & l' & l+l' \\ m & -m' & m'-m \end{pmatrix}$$

$$\times \frac{P_{l+l'}^{m-m'}(\cos\eta)}{R^{l+l'+1}} \tag{B8}$$

The special form of the Wigner 3-j symbol in this expression can be explicitly written as [16]

$$\begin{pmatrix} l & l' & l+l' \\ m & -m' & m'-m \end{pmatrix} = (-1)^{l-l'+m-m'}\left(\frac{(2l)!\ (2l')!\ (l+l'+m-m')!\ (l+l'-(m-m'))!}{(2l+2l'+1)!\ (l+m)!\ (l-m)!\ (l'-m')!\ (l'+m')!}\right)^{1/2} \tag{B9}$$

## Appendix C

This appendix presents some of the technical details in the computation of the static multipole moments. All multipole moments can be calculated analytically and no numerical integration has to be employed. This feature becomes especially advantageous in the numerical implementation of the method. The results presented in this appendix also extend to other basis functions as well. More specifically, to basis functions which are obtained by multiplying the basis functions in Section 4, Eqs.(25)-(27), by two-dimensional polynomials of arbitrary degree. Moreover, the results of this appendix extend to other polygonial shapes of subsections - not necessarily squares.

Before the explicit calculation of the static multipole moments two important tools are derived.

### Translation of the origin of a static multipole

In Section 4 the origin of the local coordinates of a subsection has been defined as the centre of the circumscribed sphere. To determine the static multipole moments we need to shift the origin of the local coordinates.

Using Eq.(A2) and the notations used in Appendix A, the dynamic multipole moment $q_n(f)$, defined by Eq.(17), can be expressed as

$$q_n(f) = \int_{V'} f(r') \, \psi_n^i(r_0') \, dv' = \sum_{n'} R_{nn'}(R) \int_{V'} f(r') \, \psi_{n'}^i(r_1')dv'$$

Denote the shifted multipole moment by $q_n(f;R)$, i.e.,

$$q_n(f;R) = \int_{V'} f(r') \, \psi_n^i(r_1')dv' \tag{C1}$$

Hence, in the dynamic case we have

$$q_n(f) = \sum_{n'} R_{nn'}(R) \, q_{n'}(f;R) \tag{C2}$$

When $kr_0' \ll 1$ we have, according to Eq.(B1) and Eq.(B4)

$$q_n(f) \rightarrow k^l \, q_n^0(f) \tag{C3}$$

and similarly when $kr_1' \ll 1$

$$q_n(f;R) \rightarrow k^l \, q_n^0(f;R) \tag{C4}$$

where the shifted static multipole moment is defined analogously to the dynamic moment. From Eqs.(C2) - (C4) we obtain

$$q_n^0(f) = \sum_{n'} R_{nn'}^0(R) \, q_{n'}^0(f;R) \tag{C5}$$

where the matrix $R_{nn'}^0$ is given by

$$R^0_{nn'} = \lim_{k \to 0} k^{l'-l} R_{nn'} = S_{nn'}(R; \lim_{k \to 0} k^{l'-l} j_\lambda) \tag{C6}$$

Taking the limit of Eq.(A7) using Eq.(B1) we find that for $l' > l$ every term of the summation in Eq.(A7) will vanish. Hence the summation in Eq.(C5) will be finite. This fact is also known from the classical theory of static multipoles [21]. When $l \geq l'$ only the term corresponding to $\lambda = l-l'$ will differ from zero. We get

$$B_{ml,m'l'}(R,\eta; \lim_{k \to 0} k^{l'-l} j_\lambda) = (-1)^{m+m'} \left( \frac{\varepsilon_m \varepsilon_{m'}}{4} \right)^{1/2} \frac{1}{(2l-2l'-1)!!}$$

$$\times \left( \frac{(2l+1)(2l'+1)(l-l'-(m-m'))!}{(l-l'+(m-m'))!} \right)^{1/2} \begin{pmatrix} l & l' & l-l' \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l & l' & l-l' \\ m & -m' & m'-m \end{pmatrix}$$

$$\times \ P^{m-m'}_{l-l'}(\cos\eta) \ R^{l-l'} \tag{C7}$$

Even permutations of the columns in the Wigner 3-j symbol do not change the value of the symbol [16], hence

$$\begin{pmatrix} l & l' & l-l' \\ m & -m' & m'-m \end{pmatrix} = \begin{pmatrix} l & l-l' & l \\ -m' & m'-m & m \end{pmatrix} \tag{C8}$$

Making the substitutions $L=l'$, $L'=l-l'$, $M=-m'$ and $M'=m-m'$ we obtain

$$\begin{pmatrix} l & l' & l-l' \\ m & -m' & m'-m \end{pmatrix} = \begin{pmatrix} L & L' & L+L' \\ M & -M' & M'-M \end{pmatrix} \tag{C9}$$

This is the same form of the Wigner 3-j symbol as in Eq.(B9).

### An integral

To determine the static multipole moments the following integral is canonical:

$$I_\sigma(\phi_0,\mu,\nu,m) = \int_0^{\phi_0} \sin^\mu\phi \cos^\nu\phi \begin{pmatrix} \cos m\phi \\ \sin m\phi \end{pmatrix} d\phi \tag{C10}$$

where $\sigma$ and $m$ are defined as in Section 3 and $\mu$ and $\nu$ are real numbers.
Using the binomial expansion theorem, the integral in Eq.(C10) can be written as

$$I_\sigma(\phi_0,\mu,\nu,m) = \int\limits_{0}^{\phi_0} \sin^\mu\phi \cos^\nu\phi \begin{pmatrix} \text{Re } e^{im\phi} \\ \text{Im } e^{im\phi} \end{pmatrix} d\phi =$$

$$= \begin{pmatrix} \sum\limits_{n=0,2,\ldots}^{m} \binom{m}{n} (-1)^{n/2} i(\phi_0,\mu+n,\nu+m-n) \\ \sum\limits_{n=1,3,\ldots}^{m} \binom{m}{n} (-1)^{(n-1)/2} i(\phi_0,\mu+n,\nu+m-n) \end{pmatrix} \tag{C12}$$

where

$$i(\phi_0,\alpha,\beta) = \int\limits_{0}^{\phi_0} \sin^\alpha\phi \cos^\beta\phi \, d\phi \tag{C13}$$

In the case when $\alpha$ or $\beta$ are integers the integral $i(\phi_0,\alpha,\beta)$ can be calculated using successive partial integrations stepping $\alpha$ or $\beta$ towards zero. In the general case the integral can be expressed as the incomplete Beta function $B_x(a,b)$ [5].

$$B_x(a,b) = \int\limits_{0}^{x} t^{a-1}(1-t)^{b-1} dt \tag{C14}$$

Using the substitution $t = \sin^2\phi$ we get

$$i(\phi_0,\alpha,\beta) = \frac{1}{2} B_{\sin^2\phi_0}((\alpha+1)/2,(\beta+1)/2) \tag{C15}$$

For our purpose the incomplete Beta function may ,e.g., be computed by the help of the hypergeometric function $_2F_1$.

$$B_x(a,b) = \frac{x^a}{a} {}_2F_1(a,1-b;a+1;x) \tag{C16}$$

## The static multipole moments

Define a local spherical coordinate system with reference to the local Cartesian coordinates in which the basis functions are expressed, cf. Fig. C1.
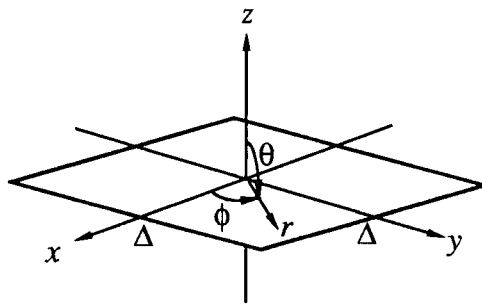


Fig. C1. The local coordinates of a subsection

The multipole moment is obtained as ($\theta=\pi/2$ )

$$q_n^0(f) = K_{ml} \int_S f_p(r) \; r^l \begin{pmatrix} \cos m\phi \\ \sin m\phi \end{pmatrix} dS \qquad \text{(C17)}$$

where the matrix $K_{ml}$ is given by

$$K_{ml} = \frac{1}{(2l+1)!!} \left( \frac{\varepsilon_m}{2\pi} \frac{2l+1}{2} \frac{(l-m)!}{(l+m)!} \right)^{1/2} P_l^m(0) \qquad \text{(C18)}$$

*Interior subsections*
Divide the integration area as shown in Fig. C2.
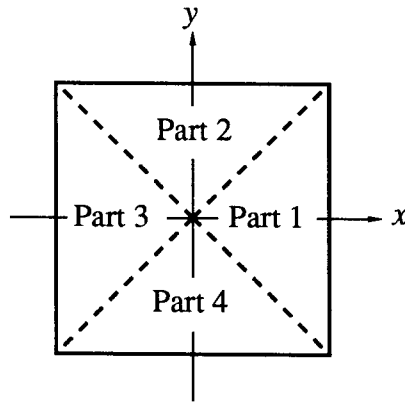


Fig. C2. The division of an interior subsection

The multipole moment of part 1 can be expressed as

$$
\begin{aligned}
q_n^0(f^l) &= K_{ml} \int_{-\pi/4}^{\pi/4} \int_0^{\frac{\Delta}{\cos\phi}} r^l \begin{pmatrix} \cos m\phi \\ \sin m\phi \end{pmatrix} r\, dr d\phi = \\
&= K_{ml} \frac{\Delta^{l+2}}{l+2} \int_{-\pi/4}^{\pi/4} \cos^{-l-2}\phi \begin{pmatrix} \cos m\phi \\ \sin m\phi \end{pmatrix} d\phi = \\
&= K_{ml} \frac{\Delta^{l+2}}{l+2} \left( I_\sigma(\pi/4, 0, -l-2, m) + I_\sigma(-\pi/4, 0, -l-2, m) \right) \qquad \text{(C18)}
\end{aligned}
$$

Obviously, the multipole moments of the other parts of the subsection can be obtained by a rotation of the part 1 moments. It is easy to show that rotating the source distribution an angle $\alpha$ in the $\phi$-direction keeping the origin fixed results in

$$q_{eml}^0(f_\alpha) = q_{eml}^0(f) \cos m\alpha - q_{oml}^0(f) \sin m\alpha \qquad \text{(C19a)}$$

$$q_{oml}^0(f_\alpha) = q_{oml}^0(f) \cos m\alpha + q_{eml}^0(f) \sin m\alpha \qquad \text{(C19b)}$$

*Edge subsections*

Using the basis function expressed by Eq.(26) we have to modify the method described above. Divide the subsection according to Fig. C3a. To calculate the moments of part 1 use shifted coordinates with the origin at point $A$ and rotated $\pi$ radians, cf. Fig. C3b.
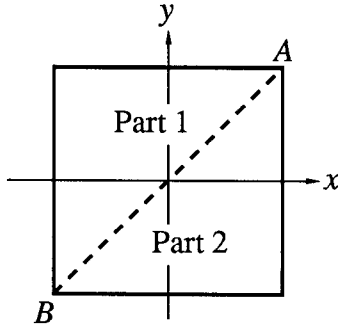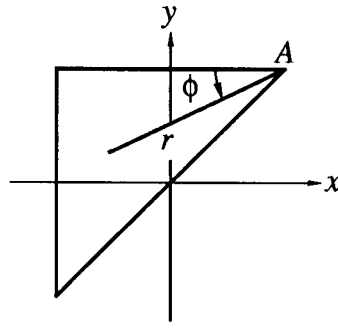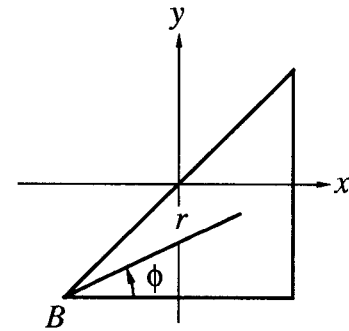


| Fig. C3a | Fig. C3b | Fig. C3c |

The division of an edge subsection and the local coordinates used in the calculations

With the notations introduced in Eq.(C1) and Eq.(C19) we get

$$q_n^0(f_\pi^E;R_A) = \kappa_{ml} \int_0^{\pi/4} \int_0^{\frac{2\Delta}{\cos\phi}} \frac{1}{\sqrt{1-(\Delta-r\cos\phi)/\Delta}} r^l \begin{pmatrix} \cos m\phi \\ \sin m\phi \end{pmatrix} r\,dr\,d\phi \tag{C20}$$

After some calculations and the use of (C12) one obtains

$$q_n^0(f_\pi^E;R_A) = \kappa_{ml} \frac{2^{l+3/2}\Delta^{l+2}}{l+3/2} I_\sigma(\pi/4,0,-l-2,m) \tag{C21}$$

Now rotate and shift the origin of the moments to the correct position at the centre of the subsection using Eq.(C19) and Eq.(C5) respectively.

The multipole moments of part 2 can be calculated using coordinates with the origin at point $B$, cf. Fig. C3c.

$$q_n^0(f^E;R_B) = \kappa_{ml} \int_0^{\pi/4} \int_0^{\frac{2\Delta}{\cos\phi}} \frac{1}{\sqrt{1-(r\cos\phi-\Delta)/\Delta}} r^l \begin{pmatrix} \cos m\phi \\ \sin m\phi \end{pmatrix} r\,dr\,d\phi \tag{C22}$$

Make the substitution $\cos^2\alpha = (r\cos\phi)/2\Delta$. The result is

$$q_n^0(f^E;R_B) = \kappa_{ml} \, 2^{l+5/2}\Delta^{l+2} \frac{(2l+2)!!}{(2l+3)!!} I_\sigma(\pi/4,0,-l-2,m) \tag{C23}$$

Now shift the origin of the moments back to the centre of the subsection using Eq.(C5). Finally add the contributions from the two parts.

*Corner subsections*

Divide the subsection as shown by Fig. C3a. To calculate the moments of part 1 use the same technique as in Eq.(C20), cf. also Fig. C3b. With the basis function given by Eq.(27) expressed in the spherical coordinates we get

$$
{}^0_n q(f_\pi^C; R_A) = \kappa_{ml} \int_0^{\pi/4} \int_0^{\frac{2\Delta}{\cos\phi}} \frac{\Delta^\lambda 2^{\lambda/2-1}}{r^\lambda} \left( \sqrt{\frac{\sin\phi}{\cos\phi}} + \sqrt{\frac{\cos\phi}{\sin\phi}} \right) r^l \binom{\cos m\phi}{\sin m\phi} r \, dr \, d\phi \qquad (C24)
$$

Straightforward calculations result in

$$
{}^0_n q(f_\pi^C; R_A) = \kappa_{ml} \frac{2^{l+1-\lambda/2} \Delta^{l+2}}{l+2-\lambda} \left( I_\sigma(\pi/4, \tfrac{1}{2}, \lambda - \tfrac{5}{2} - l, m) + I_\sigma(\pi/4, -\tfrac{1}{2}, \lambda - \tfrac{3}{2} - l, m) \right) \qquad (C25)
$$

Rotate and shift to get the desired multipole moments.
The contribution from part 2 can obviously be obtained from Eq.(C25) in a similar manner with an additional reflection.

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