Numerical Evaluation of Singular Integrands in the Application of the Charge Simulation Method with Distributed Charge Density

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Abstract: As it is well known the Charge Simulation Method is a numerical method for the computation of the electric field in three-dimensional problems, based on the concept of the substitution of the electrodic geometry with a series of elementary charge suitably arranged. In this paper we will show a possible, useful way to overpass the difficulties arising in the numerical computations on the integral expression of the electric potential in the contour points where the boundary conditions are imposed, when distributed surface charges are used in the simulation. The numerical approach presented here allows us to evaluate with accuracy the potential coefficients on the metallic surfaces, avoiding the presence of oscillatory numerical solutions in the computation of the electric potential and of the electric field strength around the electrodes, that generally occurs when discrete charges are used in the simulation.

1 Introduction

As it is well-known, the calculation of electrostatic fields requires the solution of Laplace's and Poisson's equations with the imposition of suitable boundary conditions.

Generally the geometrical complexity of the systems involved in engineering applications such as high voltage plants, power trasmission lines, makes impossible to find analytical solutions for the distribution of the electric field and its gradient strength. Therefore, numerical methods are commonly used. Among these methods, integral approaches to the solution of Laplace's and Poisson's equations, like the Charge Simulation Method ([7],[8],[3],[2],[1]), are widely used, expecially in ultra high voltage systems design, for its good applicability to full three dimensional problems. This method is based on the concept of the substitution of the electrodes geometry with a series of unknown discrete charges. The value of these charges are determined by imposing that their global effect satisfies the boundary conditions in a selected number of points, located in the boundary regions. As electric fields distribution so obtained due to these arrangements of charges satisfies the Laplace's or Poisson's equation inside the domain under analysis, the numerical solution found is unique inside the domain. The discrete nature of this approach requires the selection and the placement of a large number of fictitious charges to reach the required numerical accuracy, expecially in problems with more than two different dielectric materials and/or in presence of thin dielectric or conductors layers. Moreover, the use of discrete charges in shape of point, segment or annular sector involves their placement at a certain distance outside the boundary, to avoid singularity problems, and this fact leads to significantly loss in accuracy of the numerical computation near the interface between electrodes and dielectrics, expecially in presence of sharp edges and of thin layers of materials.

A possible way to mantain the number of the simulation charges to a practically treatable one and, at the same time, to overpass this problem, seems to be the use of distributed charge densities in the discretization.

In this paper a possible application of the Charge Simulation Method with the use of distributed charge densities, placed in the surface of the electrodes, is decribed, solving the problem of the numerical treatement of the singularities contained in the integral expression used for the evaluation of the electric potential and the field strength.

Numerical Formulation 2

In the Charge Simulation Method, for the calculation of the magnitude of the electric charges used in the discretization, n points on the surface of the conductors, called contour points, are chosen and at any of these points the electric potential resulting from the superposition of the effects of the charges is posed equal to the known boundary values:

$$V_k = \sum_{i=1}^n p_{i,k} \ q_i \tag{2.1}$$

where $p_{i,k}$ are the electric potential coefficients, q_i the distributed charges, and V_k the values of the voltage. In general, the integral expression of the coefficients $p_{i,j}$ can be written as follows:

$$p_{i,k} = \frac{1}{4\pi\epsilon |\Omega_i|} \iint_{\Omega_i} \frac{d\Omega_i}{r_{i,k}}$$
 (2.2)

where Ω_i is the portion of the surface of the electrodes where the surface charge q_i is distributed, and contain a discontinuity in the integrand functions when the i-th point coincides with the k-th one.

The numerical treatment of these discontinuity has been avoided up to now by replacing the distributed surface charges by discrete, fictitious charges, for instance in shape of point, segment, and ring. Unfortunately, numerical experiments performing this technique of arrangement have generally shown a reduction in the numerical accuracy of the results and the presence of oscillatory numerical solutions in the zones near the electrodes, where on the other hand the accurate evaluation of the electric potential and of the electric field strength are often required for the design of the devices.

In the following, a possible technique used to solve numerically the treatment of these discontinuities is described, and it is applied to the main surface portions that can be used in the numerical simulation of the behaviour of high voltage devices and systems.

Case (a). The cilindrical surface sector 2.1

Let us parametrize the cylindrical surface in cylindrical coordinates and consider the following discretization (see fig. 1):

$$h_0 = 0 < \dots < h_i < \dots < h_n = L$$
 and $\theta_0 = 0 < \dots < \theta_j < \dots < \theta_m = 2\pi$, (2.3)

where $h_i = \frac{Li}{n}$; $i = 0, \dots, n$ and $\theta_j = \frac{2\pi j}{m}$; $j = 0, \dots, m$. We will denote by $P = (R_P \cos \theta_P, R_P \sin \theta_P, h_P)$ a generic point in \mathbb{R}^3 , and by

$$P_{i,j} = \left(r\cos\frac{\theta_{j+1} + \theta_j}{2}, r\sin\frac{\theta_{j+1} + \theta_j}{2}, \frac{h_{i+1} + h_i}{2}\right) = \left(r\cos\theta^j, r\sin\theta^j, h^i\right)$$

the generic point on the cilinder's surface. The general expression for the potential coefficient $p_{(i,j),P}$ on a point P generated by the surface element $\Omega_{i,j} = \{(h,\theta) : h_i \leq h < h_{i+1}, \ \theta_j \leq \theta < \theta_{j+1}\}$ of the cilinder is:

$$p_{(i,j),P} = \frac{r}{4\pi\epsilon |\Omega_{i,j}|} \int_{\theta_j}^{\theta_j+1} \int_{h_i}^{h_{i+1}} \frac{d\theta \ dh}{\sqrt{R_p^2 + r^2 - 2R_P r \cos(\theta - \theta_P) + (h - h_P)^2}}.$$
 (2.4)

The integration with respect to the variable h can be performed in an analitical way:

setting,

$$A^{2} = R_{P}^{2} + r^{2} - 2R_{P}r\cos(\theta - \theta_{P})$$
 , $h - h_{P} = H$

we get,

$$\int \frac{dh}{\sqrt{R_P^2 + r^2 - 2R_P r \cos(\theta - \theta_P) + (h - h_P)^2}} = \int \frac{dH}{\sqrt{A^2 + H^2}}.$$
 (2.5)

Setting,

$$\sqrt{A^2 + H^2} = H + t \quad , \quad H = \frac{A^2 - t^2}{2t} \quad , \quad dH = -\frac{A^2 + t^2}{2t^2} dt$$

we have,

$$\int \frac{dH}{\sqrt{A^2 + H^2}} = -\ln t = -\ln (\sqrt{A^2 + H^2} - H). \tag{2.6}$$

By imposing the inverse substitution, we get

$$F_{j}^{P}(\theta) = \int_{h_{i}}^{h_{i+1}} \frac{dh}{\sqrt{R_{P}^{2} + r^{2} - 2R_{P}r\cos(\theta - \theta_{P}) + (h - h_{P})^{2}}}$$

$$= \ln\left(\frac{\sqrt{R_{P}^{2} + r^{2} - 2R_{P}r\cos(\theta - \theta_{P}) + (h_{i} - h_{P})^{2}} - (h_{i} - h_{P})}{\sqrt{R_{P}^{2} + r^{2} - 2R_{P}r\cos(\theta - \theta_{P}) + (h_{i+1} - h_{P})^{2}} - (h_{i+1} - h_{P})}\right)$$

$$= \ln\left(\frac{\sqrt{R_{P}^{2} + r^{2} - 2R_{P}r\cos(\theta - \theta_{P}) + (h_{i} - h_{P})^{2}} - (h_{i} - h_{P})}{R_{P}^{2} + r^{2} - 2R_{P}r\cos(\theta - \theta_{P})}\right)$$

$$+ \ln\left(\sqrt{R_{P}^{2} + r^{2} - 2R_{P}r\cos(\theta - \theta_{P}) + (h_{i+1} - h_{P})^{2}} + (h_{i+1} - h_{P})}\right)$$

with a simple rationalization.

Now, if the point P is different from $P_{i,j}$, then the integration of (2.7) with respect to θ can be performed with a simple Gaussian quadrature. For the case $P = P_{i,j}$, let us study the only singular term

$$\ln\left(2r^2(1-\cos\left(\theta-\theta^j\right)\right)\right). \tag{2.8}$$

The next step is to find the order of singularity of (2.8). To this end, let us consider

$$\lim_{\theta \to \theta^j} \frac{\ln \left(2\tau^2(1-\cos\left(\theta-\theta^j\right)\right)\right)}{\left(\frac{1}{\theta-\theta^j}\right)^{\beta}} = \lim_{\theta \to \theta^j} \frac{\sin\left(\theta-\theta^j\right)}{1-\cos\left(\theta-\theta^j\right)} \frac{(\theta-\theta^j)^{\beta+1}}{-\beta} = 0$$

for every $\beta > 0$. This means that (2.8) has a singularity of logarithmic type. Thus, we can consider the following technique as a suitable way for reducing the singularity of $F_j^{P_{i,j}}(\theta)$:

$$\int_{\theta_{j}}^{\theta_{j+1}} F_{j}^{P_{i,j}} d\theta = \int_{\theta_{j}}^{\theta^{j}} F_{j}^{P_{i,j}} d\theta + \int_{\theta^{j}}^{\theta_{j+1}} F_{j}^{P_{i,j}} d\theta
= \frac{1}{1-\gamma} \left[\int_{0}^{(\theta^{j}-\theta_{j})^{1-\gamma}} t^{\frac{\gamma}{1-\gamma}} F_{j}^{P_{i,j}} (\theta^{j} - t^{\frac{1}{1-\gamma}}) dt \right]
+ \int_{0}^{(\theta_{j+1}-\theta^{j})^{1-\gamma}} t^{\frac{\gamma}{1-\gamma}} F_{j}^{P_{i,j}} (\theta^{j} + t^{\frac{1}{1-\gamma}}) dt \right]$$
(2.9)

for any γ , with $0 < \gamma < 1$, making the change of variables $t = (\theta - \theta_j)^{1-\gamma}$ in the first integral and $t = (\theta - \theta^j)^{1-\gamma}$ in the second integral. The evaluation of these integrals is again performed by means of a Gaussian quadrature method. From our tests, it results that any γ between 0 and 1 is suitable for improving the numerical results. For the numerical simulation, we choose the value $\gamma = \frac{1}{2}$, because it is the most convenient value from a computational point of view. In fact, with $\gamma = \frac{1}{2}$, we have only to do square roots and raising to the power of two, while with $\gamma \neq \frac{1}{2}$ we have to use several routines for the raising to the power of a fractional value that are much more time consuming.

2.2 Case (b). The flat disk sector

Let us parametrize the flat disk in polar coordinates and consider the following discretization (see fig. 2):

$$\rho_0 = 0 < \dots < \rho_i < \dots < \rho_n = r \quad \text{and} \quad \theta_0 = 0 < \dots < \theta_j < \dots < \theta_m = 2\pi, \tag{2.10}$$

where $\rho_i = \frac{ri}{n}$; $i = 0, \dots, n$ and $\theta_j = \frac{2\pi j}{m}$; $j = 0, \dots, m$.

We will denote by $P = (R_P \cos \theta_P, R_P \sin \theta_P, h_P)$ a generical point in \mathbb{R}^3 , and by

$$P_{i,j} = \left(\frac{\rho_{i+1} + \rho_i}{2} \cos \frac{\theta_{j+1} + \theta_j}{2}, \frac{\rho_{i+1} + \rho_i}{2} \sin \frac{\theta_{j+1} + \theta_j}{2}, 0\right) = (\rho^i \cos \theta^j, \rho^i \sin \theta^j, 0)$$

the generic point on the flat disk. The general expression for the potential coefficient $p_{(i,j),P}$ on a point P generated by the surface element $\Omega_{i,j} = \{(\rho,\theta) : \rho_i \leq \rho < \rho_{i+1}, \ \theta_j \leq \theta < \theta_{j+1}\}$ of the flat disk is:

$$p_{(i,j),P} = \frac{1}{4\pi\epsilon |\Omega_{i,j}|} \int_{\theta_j}^{\theta_j+1} \int_{\rho_i}^{\rho_{i+1}} \frac{\rho \, d\theta \, d\rho}{\sqrt{R_p^2 + \rho^2 - 2R_P\rho\cos(\theta - \theta_P) + h_P^2}}.$$
 (2.11)

The integration with respect to the variable ρ can be performed in an analytical way:

setting,

$$A^{2} = 2R_{P}\cos(\theta - \theta_{P}) \quad , \quad B^{2} = R_{P}^{2} + h_{P}^{2}$$

$$\sqrt{\rho^{2} - A^{2}\rho + B^{2}} = \rho + t \quad , \quad \rho = \frac{B^{2} - t^{2}}{A^{2} + 2t}$$

$$d\rho = \frac{-2(t^{2} + A^{2}t + B^{2})}{(A^{2} + 2t)^{2}} dt$$

we get,

$$\int \frac{d\rho}{\sqrt{\rho^2 - A^2\rho + B^2}} = -\ln(A^2 + 2t).$$

Therefore,

$$F_{j}^{P}(\theta) = \int_{\rho_{i}}^{\rho_{i+1}} \frac{\rho \, d\rho}{\sqrt{\rho^{2} + R_{2}^{P} + h_{P}^{2} - 2\rho R_{P} \cos(\theta - \theta_{P})}}$$

$$= \frac{1}{2} \left[\int_{\rho_{i}}^{\rho_{i+1}} \frac{(2\rho - 2R_{P} \cos(\theta - \theta_{P})) \, d\rho}{\sqrt{\rho^{2} + R_{2}^{P} + h_{P}^{2} - 2\rho R_{P} \cos(\theta - \theta_{P})}} \right.$$

$$\left. - A^{2} \ln \left(2\sqrt{\rho^{2} - A^{2}\rho + B^{2}} - (2\rho - 2R_{P} \cos(\theta - \theta_{P})) \right) \right|_{\rho_{1}}^{\rho_{2}} \right]$$

$$= \frac{1}{2} \left[\sqrt{\rho_{i+1}^{2} + B^{2} - 2\rho_{i+1} R_{P} \cos(\theta - \theta_{P})} - \sqrt{\rho_{i}^{2} + B^{2} - 2\rho_{i} R_{P} \cos(\theta - \theta_{P})} \right.$$

$$\left. + A^{2} \ln \left(\frac{2\sqrt{\rho_{1}^{2} - 2R_{P}\rho_{1} \cos(\theta - \theta_{P}) + R_{P}^{2} + h_{P}^{2}} - (2\rho_{1} - 2R_{P} \cos(\theta - \theta_{P}))}{4R_{P}^{2} \sin^{2}(\theta - \theta_{P}) + 4h_{P}^{2}} \right.$$

$$\left. + A^{2} \ln \left(2\sqrt{\rho_{2}^{2} - 2R_{P}\rho_{2} \cos(\theta - \theta_{P}) + R_{P}^{2} + h_{P}^{2}} + (2\rho_{2} - 2R_{P} \cos(\theta - \theta_{P})) \right) \right]$$

with a simple rationalization.

Now, if the point P is different from $P_{i,j}$, then the integration of (2.12) in θ can be performed with a simple Gaussian quadrature. For the case $P = P_{i,j}$, proceding in analogy to the case (a), we discover that (2.12) has a singularity of logarithmic type, and a change of variables of type (2.9) with $\gamma = \frac{1}{2}$ will solve all the numerical problems due to the singularity of (2.12).

2.3 Case (c). The spherical surface sector

Let us parametrize the spherical surface in spherical coordinates and consider the following discretization (see fig. 3):

$$\phi_0 = 0 < \dots < \phi_i < \dots < \phi_n = 2\pi, \quad \text{and} \quad \theta_0 = 0 < \dots < \theta_i < \dots < \theta_m = \pi, \tag{2.13}$$

where $\phi_i = \frac{2\pi i}{n}$; $i = 0, \dots, n$ and $\theta_j = \frac{\pi j}{m}$; $j = 0, \dots, m$.

We will denote by

$$P = (R_P \sin \theta_P \cos \phi_P, R_P \sin \theta_P \sin \phi_P, R_P \cos \theta_P)$$

a generic point in \mathbb{R}^3 , and by

$$P_{i,j} = \left(r\sin\frac{\theta_{j+1} + \theta_j}{2}\cos\frac{\phi_{i+1} + \phi_i}{2}, r\sin\frac{\theta_{j+1} + \theta_j}{2}\sin\frac{\phi_{i+1} + \phi_i}{2}, r\cos\frac{\theta_{j+1} + \theta_j}{2}\right)$$
$$= \left(r\sin\theta^j\cos\phi^i, r\sin\theta^j\sin\phi^i, r\cos\theta^j\right)$$

the generical point on the spherical surface. The general expression for the potential coefficient $p_{(i,j),P}$ on a point P generated by the surface element $\Omega_{i,j} = \{(\phi,\theta): \phi_i \leq \phi < \phi_{i+1}, \ \theta_j \leq \theta < \theta_{j+1}\}$ is:

$$p_{(i,j),P} = \frac{r^2}{4\pi\epsilon \left|\Omega_{i,j}\right|} \int_{\theta_j}^{\theta_j+1} \int_{h_i}^{h_{i+1}} \frac{\sin\theta \, d\theta \, d\phi}{\sqrt{R_p^2 + r^2 - 2R_P r[\cos\theta_P \cos\theta + \cos(\phi - \phi_P)\sin\theta \sin\theta_P]}}.$$
 (2.14)

Now, if the point P is outside the finite element $\Omega_{i,j}$, then this double integral can be efficiently calculated with two nested Gaussian quadrature routines. But, if the point $P = P_{i,j}$, then the formula (2.14) becomes

$$p_{(i,j),P} = \frac{r^2}{4\sqrt{2}\pi\epsilon |\Omega_{i,j}|} \int_{\theta_j}^{\theta_j+1} \int_{h_i}^{h_{i+1}} \frac{\sin\theta \, d\theta \, d\phi}{\sqrt{1 - \left[\cos\theta_P \cos\theta + \cos\left(\phi - \phi_P\right)\sin\theta \sin\theta_P\right]}}$$
(2.15)

and the integrand

$$f_{i,j}^{P_{i,j}}(\theta,\phi) = \frac{\sin\theta}{\sqrt{1 - \left[\cos\theta_P\cos\theta + \cos\left(\phi - \phi_P\right)\sin\theta\sin\theta_P\right]}}$$
(2.16)

has a singularity in (θ^j, ϕ^i) .

For determining the order of singularity of the integration of $f_{i,j}^{P_{i,j}}$ with respect to ϕ let us proceed ad follows: setting,

$$A^2 = 1 - \cos \theta_P \cos \theta$$
 , $B^2 = \sin \theta_P \sin \theta$

(note that $A^2 - B^2 \ge 0$) we consider the change of variables

$$t=\tan\frac{\phi-\phi_P}{2},$$

$$\cos(\phi - \phi_P) = \frac{1 - t^2}{1 + t^2}$$
, $dt = \frac{1}{2}(1 + t^2) d\phi$;

Then, we have

$$\int \frac{d\phi}{\sqrt{A^2 - B^2 \cos(\phi - \phi_P)}} = \int \frac{2 \, dt}{(1 + t^2) \sqrt{(A^2 + B^2)t^2 + (A^2 - B^2)}}.$$

Again, with the change of variables

$$(A^2 - B^2) + (A^2 + B^2)t^2 = Z^2$$
 , $dt = \frac{Z dZ}{\sqrt{A^2 + B^2}\sqrt{Z^2 - (A^2 - B^2)}}$

we get

$$\int_{\phi j}^{\phi j+1} \frac{_{d\phi}}{\sqrt{_{A^2-B^2\cos(\phi-\phi_P)}}} = \int_{\sqrt{A^2-B^2}}^{\sqrt{A^2-B^2+(A^2+B^2)\tan^2\frac{\phi_{j+1}-\phi^j}{2}}} \frac{_{2\sqrt{A^2+B^2}\,dZ}}{(Z^2+2B^2)\sqrt{Z-\sqrt{A^2-B^2}}\sqrt{Z+\sqrt{A^2-B^2}}}$$

and this integral has a singularity of order $\frac{1}{2}$. The integration of $f_{i,j}^{P_{i,j}}$ between ϕ_j and ϕ^j is treated in the same way. Now, in order to determine the degree of singularity of the outer integration of (2.15), let us consider the approximation $f_{i,j}^1$ of $f_{i,j}^{P_{i,j}}$ given by:

$$f_{i,j}^{1}(\theta,\phi) = \frac{\sin\theta}{\sqrt{1-\cos\theta^{j}\cos\theta - \sin\theta\sin\theta^{j} + \sin\theta\sin\theta^{j} \frac{(\phi-\phi^{i})^{2}}{2}}}$$
(2.17)

Now, we know how to integrate analytically $f^1_{i,j}$ with respect to ϕ :

setting,

$$A^2 = 1 - \cos\theta \cos\theta^j - \sin\theta \sin\theta^j$$
 , $B^2 = \frac{\sin\theta \sin\theta^j}{2}$, $Z = \phi - \phi^i$

we consider the change of variables

$$\sqrt{A^2 + B^2 Z^2} = BZ + t,$$

$$Z = \frac{A^2 - t^2}{2Bt} , \quad dZ = -\frac{1}{2B} \frac{A^2 + t^2}{t^2} dt;$$
(2.18)

Then, we have

$$\int \frac{dZ}{\sqrt{A^2 + B^2 Z^2}} = -\frac{1}{B} \ln \left(\sqrt{A^2 + B^2 Z^2} - BZ \right).$$

Therefore,

$$\begin{split} F_{i,j}^1 &= \int_{\phi_i}^{\phi_{i+1}} f_{i,j}^1(\theta,\phi) \, d\phi \\ &= \frac{\sin \theta}{\sqrt{\frac{\sin \theta \sin \theta^j}{2}}} \left[\ln \left(\frac{\sqrt{1 - \cos \theta \cos \theta^j - \sin \theta \sin \theta^j + \sin \theta \sin \theta^j \frac{(\phi_i - \phi^i)^2}{2}} - B(\phi_i - \phi^i)}{[1 - \cos (\theta - \theta^j)]} \right) \\ &+ \ln \left(\sqrt{1 - \cos \theta \cos \theta^j - \sin \theta \sin \theta^j + \sin \theta \sin \theta^j \frac{(\phi_{i+1} - \phi^i)^2}{2}} + B(\phi_{i+1} - \phi^i)} \right) \right] \end{split}$$

Following the same analitical procedures described in the case (a), we can prove that this function has a singularity of logarithmic type in $\theta = \theta^j$. These results allow us to consider the following change of variables as a possible and suitable way for reducing the singularity of the double integral in (2.15):

$$F_{i,j}^{P_{i,j}}(\theta) = \int_{\phi_i}^{\phi_{i+1}} f_{i,j}^{P_{i,j}}(\theta,\phi) d\phi$$

$$= \int_{0}^{\sqrt{\frac{\phi^i - \phi_i}{2}}} 2t f_{i,j}^{P_{i,j}}(\theta,\phi^i - t^2) dt + \int_{0}^{\sqrt{\frac{\phi_{i+1} - \phi^i}{2}}} 2t f_{i,j}^{P_{i,j}}(\theta,\phi^i + t^2) dt;$$
(2.19)

$$\int_{\theta_{i}}^{\theta_{j+1}} F_{i,j}^{P_{i,j}}(\theta) d\theta = \int_{0}^{\sqrt{\frac{\theta^{j-\theta_{j}}}{2}}} 2t F_{i,j}^{P_{i,j}}(\theta^{j} - t^{2}) dt + \int_{0}^{\sqrt{\frac{\theta_{j+1} - \theta^{j}}{2}}} 2t F_{i,j}^{P_{i,j}}(\theta^{j} + t^{2}) dt.$$
 (2.20)

Case (d). The annular surface sector

Let us parametrize the annular surface in the following way:

$$x = (R - r \cos \theta) \cos \phi$$

$$y = (R - r \cos \theta) \sin \phi$$

$$z = r \sin \theta$$
(2.21)

and consider the following discretization (see fig. 4):

$$\phi_0 = 0 < \dots < \phi_i < \dots < \phi_n = 2\pi \quad \text{and} \quad \theta_0 = 0 < \dots < \theta_i < \dots < \theta_m = 2\pi, \tag{2.22}$$

where $\phi_i = \frac{2\pi i}{n}$; $i = 0, \dots, n$ and $\theta_j = \frac{2\pi j}{m}$; $j = 0, \dots, m$. We indicate as $P = ((R_P - r_P \cos \theta_P) \cos \phi_P, (R_P - r_P \cos \theta_P) \sin \phi_P, r_P \sin \theta_P)$ a generical point in \mathbb{R}^3 , and by

$$\begin{split} P_{i,j} &= \left((R - r\cos\frac{\theta_{j+1} + \theta_{j}}{2})\cos\frac{\phi_{i+1} + \phi_{i}}{2}, (R - r\cos\frac{\theta_{j+1} + \theta_{j}}{2})\sin\frac{\phi_{i+1} + \phi_{i}}{2}, r\sin\frac{\theta_{j+1} + \theta_{j}}{2} \right) \\ &= \left((R - r\cos\theta^{j})\cos\phi^{i}, (R - r\cos\theta^{j})\sin\phi^{i}, r\sin\theta^{j} \right) \end{split}$$

the generical point on the annular surface. The general expression for the potential coefficient $p_{(i,j),P}$ on a point P generated by the surface element $\Omega_{i,j} = \{(\phi,\theta): \phi_i \leq \phi < \phi_{i+1}, \ \theta_j \leq \theta < \theta_{j+1}\}$ of the torus is:

$$p_{(i,j),P} = \frac{r}{4\pi\epsilon |\Omega_{i,j}|} \int_{\theta_i}^{\theta_j+1} \int_{\phi_i}^{\phi_{i+1}} \frac{(R - r\cos\theta) d\theta d\phi}{\|P_{i,j} - P\|}$$
(2.23)

Now, if the point P is outside the finite element $\Omega_{i,j}$, this double integral can be efficiently calculated with two iterated Gaussian quadrature.

But, if the point $P = P_{i,j}$, then the formula (2.23) becomes

$$p_{(i,j),P} = \frac{r}{4\pi\epsilon |\Omega_{i,j}|} \int_{\theta_{i}}^{\theta_{j}+1} \int_{\phi_{i}}^{\phi_{i+1}} \frac{(R - r\cos\theta) d\theta d\phi}{\sqrt{2(R - r\cos\theta)^{2}[1 - \cos(\phi - \phi^{1})] + r^{2}(\sin\theta - \sin\theta^{2})^{2}}}$$
(2.24)

and the integrand

$$f_{i,j}^{P_{i,j}}(\theta,\phi) = \frac{(R - r\cos\theta)}{\sqrt{2(R - r\cos\theta)^2[1 - \cos(\phi - \phi^i)] + r^2(\sin\theta - \sin\theta^j)^2}}$$
(2.25)

has a singularity in (θ^j, ϕ^i) .

As we did in the case (c), in order to determine the degree of singularity of the outer integration of (2.24), let us consider the approximation $f_{i,j}^1$ of $f_{i,j}^{P_{i,j}}$ given by:

$$f_{i,j}^{1}(\theta,\phi) = \frac{(R - r\cos\theta)}{\sqrt{(R - r\cos\theta)^{2}(\phi - \phi^{i})^{2} + r^{2}(\sin\theta - \sin\theta^{j})^{2}}}$$
(2.26)

Now, by operating in analogy with the case (c), we find that the iterated integrations in (2.24) have the same order of singularity as in the spherical case, and therefore we can reduce the singularity of the double integral in (2.24) with two changes of variables as we did in (2.19) and (2.20).

3 Numerical Tests

Taking into account the shape of the integrand functions, we used the Gauss-Legendre quadrature method for the numerical computation of the potential coefficients.

As it is well known, the choice of the number of weights and points used in the quadrature routines is a critical point. To this purpose, we have to distinguish the evaluation of the potential coefficients containing a singularity from those having no singularity. In absence of singularity, that is when $i \neq k$ in (2.1), few points are sufficient for a good numerical approximation; we found that 8 points for each step of integration are more than sufficient for an accuracy of 6 or more digits. In presence of a singularity, it is expected a sensible growth of the number of points needed for an accurate numerical integration, although the change of variables of the type (2.19) and (2.20) remove the singularity from an analytical point of view. In fact, the quadrature routine must evaluate the product of two critical terms: one very small and the other very large. Even if this product has a finite value, the evaluation is not very stable from a numerical point of view.

The table 1 shows how the quadrature routines (we use a routine in [4] for the generation of the weights and points) behave in the four cases (a)-(d). The quadrature routines works in double precision. The execution time is referred to a Pentium 90 MHz processor. We estimated the degree of precision by comparison with the analytical solution when it exists (i.e. the case of the insulated whole spherical surface), elsewhere by taking into account the number of digits that remain unchanged when a large number of weights and points in the Gauss-Legendre quadrature routines is used.

the execution time is quite short, bearing in mind the plain hardware computer board used. The first accuracy and execution time results are related to the routines implementing the change of variables, the second without the change of variables. It is straightforward to derive that by using our method the accuracy in the calculations is significantly better and the time needed reasonably contained.

It should be underlined that it is convenient to use a limited number of points in the Gauss-Legendre quadrature routines, as shown in table 1. This fact occurs for two reasons: first, the increasing of the number of points does not affect significantly the accuracy, but it increases the computational time; secondly, if we take a large number of points there is the risk that the numerical results of some operations in the calculation may have overflow and underflow problems. For example, referring to table 1, we found that numerical problems occurred when we used more than 130 points.

Table 1: Numerical tests.

Sector Type	N. of points for	N. of points for	Accuracy		Execution	
	outer integration	inner integration	Digits		time in ms.	
			with	without	with	without
Cilinder		8	4	1	< 10	< 10
and	******	16	5	1	< 10	< 10
Flat Disk	_	32	6	2	< 10	< 10
	_	64	8	3	< 10	< 10
	_	128	8	3	< 10	< 10
Sphere	8	16	3	1	< 50	< 50
and	16	16	4	1	< 50	< 50
Annulus	16	32	5	2	< 50	< 50
	16	64	5	2	< 50	< 50
	32	32	5	2	< 50	< 50
	32	64	6	2	50	< 50
	64	64	6	2	220	110
	64	128	6	2	320	170
	100	128	7	2	550	305

4 Conclusions

In this paper a possible, useful numerical approach to the accurate evaluation of the potential coefficients in integral methods, such as the Charge Simulation Method taking into account surface distributed charges is shown.

The approach consists in a complete mathematical study of the integral singularity resulting in a suitable change of variables, whose effects is to reduce the singularity from an analitical point of view. Following this approach, degrees of precision of six or more digits can be easily obtained and the numerical accuracy of the electrostatic analysis may be conveniently improved expecially in critical zones, such as near the electrodes, in presence of sharp edges or of thin dielectric layers. Of course, further developments and more detailed numerical tests dealing with practical engineering problems are opportune and necessary.

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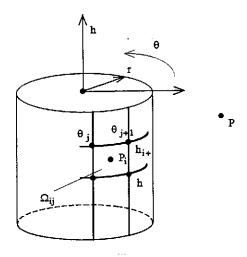


Fig. 1 - The cylindrical surface sector.

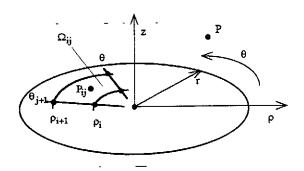


Fig. 2 - The flat disk sector.

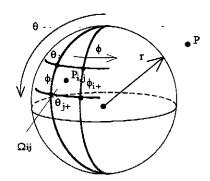


Fig. 3 - The spherical surface sector.

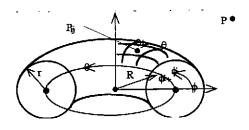


Fig. 4 - The annular surface sector.