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Note

Solution of the Discrete Poisson Equation with Complicated Boundaries

1. INTRODUCTION

Very fast exact direct methods now exist for the direct solution of the discrete Poisson equation in rectangular [1, 2] or cylindrical domains [3]. For more complicated domains, Hockney [1] and Buzbee *et al.* [4] treat the walls as long electrodes inside a regular domain and apply the "Capacity Matrix" method. If P grid points represent the electrodes on the finite difference grid, one first solves for the potential with no charge on these P points. A P-vector is formed with the potential missing on the electrodes and multiplied by the P-order capacity matrix to obtain the induced charge P-vector. Adding this to the original charge distribution and solving again gives the desired potential.

While the method is exact and quite rapid (approximately 2Θ, where Θ is the time required for a solution in the simple domain), and the capacity matrix need be computed only once (it depends only on the position of the electrodes), its calculation can be burdensome in the study of large systems or for users of modest computer installations: the computing time required is $P\Theta$ [4], and the storage space P^2.

A coarse grid reduces both P and Θ but, in plasma simulations, grid spacings much larger than a Debye length are not acceptable [5]. In three-dimensional computations, Θ is large and finite area electrodes would also make P large, thus precluding the application of the method.

It is therefore desirable to reduce the value of P, even at some expense in accuracy, to get a more manageable capacity matrix.

Fortunately, examination of the distribution of induced charge along lengthy electrodes shows that it varies slowly and smoothly except at the ends. (This is less so for electrodes which are oblique with respect to the coordinate axes. This particular problem is discussed in Section 3). This suggests the grouping of electrode points into clusters, and simply demanding that the *average* potential on each cluster be the electrode potential. The error made is the deviation from the mean of the potential on the points in the clusters, and we show how an appropriate prescription for computing the induced charge in the clusters can make this error extremely small. Numerical results are given for a potential calculation on the KEMP–II plasma confinement machine.

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2. Numerical Method

To simplify, we will consider only one long electrode with P grid points to be held at potential v^{EL}. The extension to more than one electrodes is obvious. These P points are grouped into M clusters, each of which includes η_m points ($\eta_m \geqslant 1$, $m = 1,..., M$). Let l_p designate the coordinate of the pth electrode grid-point ($p = 1, 2,..., P$) and l_{m1}, l_{m2}, etc., that of the first, second, etc., point of the mth cluster. Only one index indicates the coordinate on a two-dimensional grid:

$$l = i + j*NZ.$$

As the charge varies rapidly at either end of the electrode, we use one point clusters near the ends

$$\eta_1 = \cdots = \eta_{NI} = 1; \qquad \eta_{M-NF+1} = \cdots = \eta_M = 1. \tag{1}$$

Usually, NI and NF are 3 or 4. For the other clusters, $\eta_m > 1$, usually 2, 3, or 4.

We must always have

$$\sum_{m=1}^{M} \eta_m = P. \tag{2}$$

We define M basic density distributions which will be used to expand the distribution of induced charges

$$\rho^I = \sum_{m=1}^{M} q_m \hat{\rho}_m .$$

For one-point clusters, we define a distribution which is unity on the one-point cluster, and null elsewhere

$$(\hat{\rho}_m)_l = \delta_{l,l_{m1}}, \qquad 1 \leqslant m \leqslant NI \quad \text{or} \quad M - NF + 1 \leqslant m \leqslant M. \tag{3}$$

For the M' ($M' = M - NI - NF$) other clusters, we use polynomials of degree $(M' - 1)$ in $x_{l_{mk}}$, the projected distance between the beginning of the electrode and point l_{mk} ($x_{l_{11}} \equiv 0$)

$$\begin{aligned} (\hat{\rho}_m)_l &= 0 \text{ if } l \text{ is a point which is on a one point cluster or is not on the electrode,} \\ &= F_m(x_l) \text{ if } l = l_{mk} \text{ is a point in a multipoint cluster,} \end{aligned} \tag{4}$$

where

$$F_m(x_{l_{mk}}) = \prod_{\substack{n=NI+1 \\ n \neq m}}^{M-NF} \frac{(x_{l_{mk}} - x_{l_{n1}})}{(x_{l_{m1}} - x_{l_{n1}})} . \tag{5}$$

It may be verified that the induced charge is q_m on the first point of cluster m and, on the other points, is established by M'-pivotal points Lagrangian interpolation [8].

The calculation of the capacity matrix now proceeds as follows.

(a) Compute the "average potentials matrix" $\boldsymbol{D}$.

For $m = 1, 2,..., M$,

(i) solve the Poisson equation with density $\hat{\rho}_m$.

$$\Psi_m = \boldsymbol{L}^{-1}\hat{\rho}_m , \tag{6}$$

where $\boldsymbol{L}$ is the finite difference Poisson operator for the simple geometry, and $\boldsymbol{L}^{-1}$, its inverse, refers to the direct solution method;

(ii) form the average potentials M-vector (averaging on each cluster). This vector is the mth row of matrix $\boldsymbol{D}$

$$d_{mn} = (1/\eta_n)[(\Psi_m)_{l_{n1}} + \cdots + (\Psi_m)_{l_{nn_n}}] \qquad (n = 1, 2,..., M). \tag{7}$$

(b) Invert the $M \times M$ matrix $\boldsymbol{D}$ to obtain the capacity matrix

$$\boldsymbol{C} = \boldsymbol{D}^{-1}. \tag{8}$$

The calculation of the potential for a given charge density off the electrodes, ρ^0, proceeds as follows.

(a) Compute the potential with no charge on the electrodes

$$\Phi^0 = \boldsymbol{L}^{-1}\rho^0. \tag{9}$$

(b) Form the "missing average potential" M-vector $\mathbf{U}$

$$u_m = v^{\mathrm{EL}} - (1/\eta_m)[(\Phi^0)_{l_{m1}} + \cdots + (\Phi^0)_{l_{mn_n}}] \qquad (m = 1,..., M). \tag{10}$$

(c) Multiply this vector by the capacity matrix $\boldsymbol{C}$ to obtain the missing charge M-vector $\mathbf{Q}$

$$\mathbf{Q} = \boldsymbol{C}\mathbf{U}. \tag{11}$$

(d) Add the induced charge to the given charge distribution

$$\rho = \rho^0 + \rho^{\mathrm{I}} = \rho^0 + \sum_{m=1}^{M} q_m\hat{\rho}_m . \tag{12}$$

(e) Solve the Poisson equation with this charge distribution

$$\Phi = \boldsymbol{L}^{-1}\rho. \tag{13}$$

It can be proved that the potential thus obtained has exactly the correct average potential on each cluster

$$(1/\eta_m)[(\Phi)_{l_{m1}} + \cdots + (\Phi)_{l_{m\eta_m}}] = v^{\mathrm{EL}}. \tag{14}$$

3. Oblique Electrodes

When an oblique electrode is represented on a finite difference grid, it generally takes a jagged, staircase-like form and it is found, if the induced charge is calculated exactly, that considerably more charge is induced on the corners of the "staircase" than on the neighboring points. This is not well approximated by the polynomials used to calculate the induced charge, but we have found empirically that this difficulty is considerably alleviated by weighing the polynomials with the distance between two points; that is, we replace Eq. (4) by

$$(\hat{\rho}_m)_{l_{mk}} = F_m(x_{l_{mk}})(x_{l_{mk+1}} - x_{l_{mk}}). \tag{15}$$

However, even this weighing does not succeed completely in making the clustering approximation equally good for oblique electrodes as compared to horizontal or vertical ones.

4. Numerical Test

To test the clustering method, we have applied it to the study of the KEMP–II (electrostatic and magnetic confinement) experimental facility (Fig. 1). A potential distribution obtained from an iterative equilibrium calculation [6] was used as a basis for comparison. The charge distribution was calculated directly by the finite difference Poisson equations and input to the direct solution code. Comparison of the potential thus obtained with the original potential, near and on the electrodes permits an evaluation of the accuracy of the clustering approximation (Table I).

In this example, a nonuniform grid spacing in the radial direction is used to improve resolution near the axis. The potential in the simple half-cylinder is obtained from the density by Fourier transformation in the axial direction and Gaussian elimination in the radial direction [3, 7]. The grid is 64×100 cells.

While the electrodes A and B were treated exactly ($\eta_m = 1$), the walls were treated approximately with $\eta_m = 3$, $NI = NF = 4$ for all three walls: W1, W2, W3. The 118 points to be held at fixed potential were thus grouped in 69 clusters, for a nearly twofold reduction in the computer time necessary to calculate the capacity matrix, and a threefold reduction in its storage space.

The worst error appears on wall W2, as the latter is oblique.

The worst error is given, for each wall, in volts and as a percentage of the voltage applied on it (6000 volts). The comparisons near the walls are made 2(5) grid spacings below W1 and 2(5) grid spacings right of W2 and W3.

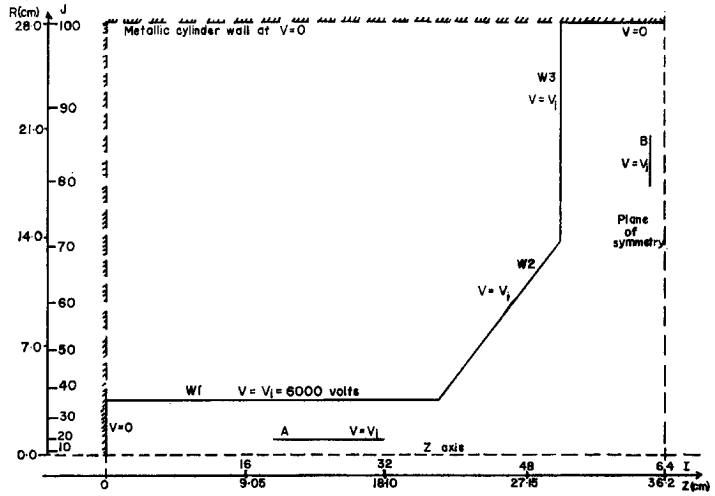

FIG. 1. Model of the KEMP–II plasma confinement machine

TABLE I

Precision of the Algorithm for the KEMP–II Plasma Machine

Wall	Number of grid-points P	Number of clusters M	Worst error on the wall (V; %)	Worst error 2 points from the wall (V; %)	Worst errors 5 points from the wall (V; %)
W1	40	20	2.5 0.042%	0.96[a] 0.016%	0.34[a] 0.0057%
W2	33	17	11.4 0.19%	5.2 0.087%	3.5 0.058%
W3	29	16	0.2 0.0035%	0.12[a] 0.0020%	0.15[a] 0.0025%

[a] The 5 points below (right of) W1 (W3) closest to W2 were excluded from this comparison as the error there is due to the error on W2, and not to that on W1 (W3).

5. Conclusion

The clustering method permits an appreciable reduction in computer time and storage space at a small cost in the accuracy of potential calculations. In the case outlined above, the worst error on the oblique wall was less than 0.2% and this fell off to below 0.1% only two grid spacings away from the wall. The precision was five times better on and close to the nonoblique walls. Thus, if one desired this much more precision, one would not apply the clustering approximation to the oblique wall, which would, however, increase the number of clusters from 69 to 85. A compromise between accuracy and computer time and space must, as usual, be made.

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Jean-Pierre Matte
Gaétan Lafrance

INRS–Energie
Université du Québec
C. P. 1020, Varennes
Québec, JOL 2PO, Canada

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