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LETTER TO THE EDITOR

Electrostatic boundary corrections for unscreened point charges

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Abstract. We present a 'correction' method to match electrostatic boundary conditions for the Poisson equation in the presence of unscreened interior point charges. This method is applicable to any general electrostatic boundary conditions, is independent of the geometry of the boundaries, and is well suited to numerical computation. It is based on correcting the changes in boundary values caused by the presence of the point charges. Thus, the corrected boundary conditions include not only the effects of all exterior charges, but also the effects of the interior point charges.

Boundary conditions are frequently used in the solution of electrostatic problems to replace the complicated effects of charges located outside the boundaries. Many standard techniques exist for solving the Poisson equation while matching the boundary conditions to obtain unique solutions to the problem. The matching of these boundary conditions can be difficult in situations where point charges are included within the boundaries. A popular method used to compute the long-range Coulomb potential of a collection of point charges within boundaries is the method of images, which uses the Ewald summation technique [1, 2].

We present here an alternative 'correction' method. This method is applicable to any general electrostatic boundary conditions, is independent of the geometry of the boundaries, and is well suited to numerical computation. It is based on correcting the changes in boundary values caused by the presence of the interior point charges.

The 'correction' method was applied [3, 4] in a 'molecular dynamics' [5] simulation of the dynamically correlated scattering of unscreened mobile point charges. These mobile charges scattered from each other and from fixed point charges.

The electrostatic potential everywhere within a volume is uniquely determined by the charge distribution within the volume and by the boundary conditions at the surface (see any standard textbook on electricity and magnetism, also [6]). These boundary conditions are specified in terms of either the electrostatic potential at the surface, or the normal component of the electric field thereon.

If the electric charge within the volume is everywhere zero, the potential inside is found from the particular (unique) solution of the (source-free) Laplace equation within the volume, which also satisfies the boundary conditions specified at the surface.

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If the electric charge within the volume consists of a finite charge density $\rho(x, y, z) = \rho(\boldsymbol{r})$, then one proceeds in a similar fashion. One chooses from the solutions of the Poisson equation for the given charge (source) density within the volume, the (unique) solution which satisfies the given boundary conditions at the surface.

That part $U_1(\boldsymbol{A})$ of the electrostatic scalar potential $U(\boldsymbol{A})$ at a point $\boldsymbol{A} = (A_x, A_y, A_z)$, which is due only to point charges of charge Q_j at points $\boldsymbol{r}_j = (x_j, y_j, z_j)$ inside the volume, is found from the sum of the individual Coulomb potentials of the interior point charges, Q_j, where ε is the permittivity of the medium,

$$U_1(\boldsymbol{A}) = \sum_j (Q_j/4\pi\varepsilon|\boldsymbol{A} - \boldsymbol{r}_j|). \tag{1}$$

This potential $U_1(\boldsymbol{A})$ is in fact a solution to the Poisson equation with delta function sources at points $\boldsymbol{r}_j$.

That part $U_2(\boldsymbol{A})$ of the electrostatic scalar potential at a point $\boldsymbol{A} = (A_x, A_y, A_z)$ inside the volume, which is due only to charges on and outside the surface of the volume, could be found in the same way as for interior charges, if the positions and strengths of all external charges were known. However, the positions of the external and/or surface charges are changed when the positions and/or strengths of the interior charges are changed.

If the electrostatic scalar potential $U(\boldsymbol{B})$ at all boundary points $\boldsymbol{B} = (B_x, B_y, B_z)$ is specified as a boundary condition

$$U(\boldsymbol{B}) = U_{\mathrm{B}}(\boldsymbol{B}) \tag{2}$$

(as is usually done for conducting boundaries) then one is tempted to seek a solution by adding (linear superposition) to the potential U_1 of (1), the potential U_2 found by solving the Laplace equation subject to the boundary potential $U_B(\boldsymbol{B})$. However, the potential at the surface would then be $U(\boldsymbol{B}) = U_{\mathrm{B}}(\boldsymbol{B}) + U_1(\boldsymbol{B})$. To 'correct' for this error, we seek instead the potential U_2 found by solving the Laplace equation subject to the boundary potential

$$U_2(\boldsymbol{B}) = U_{\mathrm{B}}(\boldsymbol{B}) - U_1(\boldsymbol{B}). \tag{3}$$

The potential $U(\boldsymbol{A})$

$$U(\boldsymbol{A}) = U_1(\boldsymbol{A}) + U_2(\boldsymbol{A}) \tag{4}$$

is thus a solution of the Poisson equation everywhere inside the volume for the given sources. From (3) and (4) we see that it has the correct value

$$U(\boldsymbol{B}) = U_1(\boldsymbol{B}) + U_2(\boldsymbol{B}) = U_1(\boldsymbol{B}) + U_{\mathrm{B}}(\boldsymbol{B}) - U_1(\boldsymbol{B}) = U_{\mathrm{B}}(\boldsymbol{B}) \tag{5}$$

at the surface. Hence, it is the unique solution of the problem.

If instead of the potential $U_{\mathrm{B}}(\boldsymbol{B})$ at the boundary, its normal gradient at some or all boundary points $\boldsymbol{B} = (B_x, B_y, B_z)$ is specified as a boundary condition (as is usually done for boundaries of high symmetry) then one can proceed in a very similar way. Since the electrostatic field is found from

$$\boldsymbol{E} = -\mathrm{grad}\ \boldsymbol{U} \tag{6}$$

it is $E_{\mathrm{n}}(\boldsymbol{B})$, the normal (n) component of $\boldsymbol{E}$ evaluated at those boundary points $\boldsymbol{B}$ which is specified.

We seek now the potential U_2 found by solving the Laplace equation subject to the boundary potential

$$U_2(\boldsymbol{B}) = U_{\mathrm{B}}(\boldsymbol{B}) - U_1(\boldsymbol{B}) \tag{7}$$

wherever the boundary potential is specified, and subject to

$$E_{\mathrm{n}2}(\boldsymbol{B}) = E_{\mathrm{nB}}(\boldsymbol{B}) - E_{\mathrm{n}1}(\boldsymbol{B}) \tag{8}$$

wherever the normal gradient of the boundary potential is specified. These correction terms $-U_1(\boldsymbol{B})$ and $-E_{\mathrm{n}1}(\boldsymbol{B})$ ensure that the total potential $U(\boldsymbol{A})$ of (4) matches the specified mixed boundary conditions.

If the electric charge within the volume consists of both point charges and a finite distributed charge density $\rho(x, y, z) = \rho(\boldsymbol{r})$, then one proceeds in a manner similar to that described above. However, one now solves the Poisson equation (instead of the Laplace equation) for U_2, taking into account only the distributed charge density (without the point charges) and subject to the boundary conditions corrected for the interior point charges. The total potential $U(\boldsymbol{A})$ of (4) is then a solution of the Poisson equation for all the charges in the interior, and matches the specified mixed boundary conditions.

Our method may be summarised as follows. The unique electrostatic potential for a closed system of point charges and distributed charge density, for the case of general mixed boundary conditions, is found from

$$U(\boldsymbol{A}) = U_1(\boldsymbol{A}) + U_2(\boldsymbol{A}) \tag{4}$$

where $U_1(\boldsymbol{A})$ is the potential due to the interior point charges alone,

$$U_1(\boldsymbol{A}) = \sum_j (Q_j/4\pi\varepsilon|\boldsymbol{A} - \boldsymbol{r}_j|) \tag{1}$$

and $U_2(\boldsymbol{A})$ is the potential found from the solution of the Poisson equation, neglecting the interior point charges, and replacing the actual boundary conditions, $U(\boldsymbol{B}) = U_{\mathrm{B}}(\boldsymbol{B})$ and $E_{\mathrm{n}}(\boldsymbol{B}) = E_{\mathrm{nB}}(\boldsymbol{B})$, by 'corrected' boundary values:

$$\text{'corrected' } U(\boldsymbol{B}) = U_{\mathrm{B}}(\boldsymbol{B}) - U_1(\boldsymbol{B}) \tag{7$'$}$$

$$\text{'corrected' } E_{\mathrm{n}}(\boldsymbol{B}) = E_{\mathrm{nB}}(\boldsymbol{B}) - E_{\mathrm{n}1}(\boldsymbol{B}). \tag{8$'$}$$

The 'correction' method for solving electrostatic boundary value problems in the presence of point charges provides a simple use of linear superposition. The solution may be found from the Coulomb potential of the point charges, added to the solution of the Poisson equation 'neglecting' the point charges in the source term. The 'error' caused by 'neglecting' the point charge source terms is 'corrected' by modifying the boundary potential or the normal component of the boundary electric field. This procedure has the advantage over image methods, in that it allows for the use of the usually very efficient Poisson equation solvers without modification.

We see that our 'correction' method is a natural extension of the general philosophy of using boundary conditions. Traditionally, one replaces the effects of all the exterior charges by boundary conditions; in our 'correction' technique, we replace the effects of these exterior charges and the effects of the interior point charges by 'corrected' boundary conditions.

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