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Remarks on the Numerical Solution of Poisson's Equation for Isolated Charge Distributions*

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A method is proposed to provide an efficient correction to the potential and field of an isolated charge distribution calculated by means of the Fourier transform technique. The method also applies to other problems involving Poisson's or Yukawa's equation for isolated sources.

The numerical treatment of many physical systems requires the repeated solution of an equation of the type

$$\Delta\phi(\mathbf{r}) - \alpha^2\phi(\mathbf{r}) = \rho(\mathbf{r}) \tag{1}$$

with ρ given on some discrete number of mesh points in two- or three-dimensional space. For $\alpha = 0$ this is just Poisson's equation which determines the electric potential ϕ of a charge distribution ρ or the gravitational potential of some arrangement of masses. Thus, there are immediate applications in the numerical treatment of charged fluids, plasmas, and galaxies [1]. In addition, the implicit formulation of time-dependent differential equations may require the solution of an equation of this type to get the physical quantity being time-stepped at an advanced time [2]. Finally, for $\alpha \neq 0$, Eq. (1) determines the Yukawa potential of an assembly of nuclear matter, which makes it useful in nuclear physics even aside from the calculation of Coulomb potentials.

Several methods have been developed to solve Eq. (1) numerically in the two-dimensional case, and they may be classified coarsely according to their use of fast Fourier transform (FFT) methods [3] as opposed to purely algebraic techniques. The straightforward FFT approach replaces Eq. (1) by its Fourier-transformed analog

$$-(2\pi/N)^2\,\mathbf{k}^2\tilde{\phi}(\mathbf{k}) + \alpha^2\tilde{\phi}(\mathbf{k}) = \tilde{\rho}(\mathbf{k}) \tag{2}$$

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with

$$\tilde{\phi}(\mathbf{k}) = \sum_{\mathbf{r}} \phi(\mathbf{r}) \exp[2\pi i \mathbf{r} \cdot \mathbf{k}/N] \tag{3}$$

and analogously for $\tilde{\rho}$. To simplify the notation, it was assumed that $\mathbf{r}$ and $\mathbf{k}$ vary on a mesh of $N \times N \times N$ points (N even) with a mesh size of a for $\mathbf{r}$ and a^{-1} for $\mathbf{k}$, and each component runs over all values k times mesh size with $k = -N/2, -N/2 + 1, \ldots, N/2 - 1$.

Now Eq. (2) may be solved easily for the Fourier components $\tilde{\phi}(\mathbf{k})$ and transforming back into coordinate space yields the potential ϕ.

In two dimensions, however, it is advantageous to combine a FFT in one dimension with an algebraic reduction method in the other dimension, as exemplified by Hockney's FACR algorithm [4], or to use algebraic methods throughout, as does Buneman's direct cyclic reduction algorithm [5]. These are about a factor of 2 faster than the FFT method.

For three dimensions, on the other hand, the FFT approach tends to gain somewhat in attractiveness, because it is easiest to generalize and because of the small number of mesh points N in each dimension, which for the present generation of computers cannot easily transcend 64, the FFT algorithm involves many multiplications with trivial factors like 1 or -1 which can be avoided by judicious programming.

There is, however, another drawback to the FFT method, and that is its inflexibility with respect to boundary conditions. The only boundary condition that can be treated efficiently is that corresponding to a periodic repetition of source ρ and potential ϕ in all three dimensions. Thus, even the simple case of an isolated source with the potential going to zero at infinity cannot be treated directly.

For dealing with this case Hockney [1] recommends surrounding the charge distribution with empty areas on all sides by doubling the number of mesh points in each dimension and setting $\rho = 0$ on the additional points. Thus, in two dimensions the rectangle containing the charges is surrounded by three empty rectangles of the same size, so that the number of grid points increases by a factor of 4. In three dimensions the same procedure leads to an eightfold increase in the number of points, which aggravates time and storage problems considerably.

The essence of this method is to keep the unrealistic boundary conditions, but reduce their influence in the region of interest by moving the boundaries further away. We shall refer to this method as the "empty-cell method."

The method we are proposing proceeds quite differently: We keep the boundaries relatively close to the charge distribution, but subtract the influence of its periodic repetitions in some given approximation, so that the accuracy of the solution is increased considerably.

To that end, we note that the Fourier transform $\tilde{\rho}(\mathbf{k})$ of a given charge distribution $\rho(\mathbf{r})$ will correspond to a periodic repetition of $\rho(\mathbf{r})$, if it is transformed

back into coordinate space and taken to be valid outside the original cell as well. So it actually describes the periodic charge distribution

$$\rho_{\text{per}}(\mathbf{r}) = \sum_{\mathbf{n}} \rho(\mathbf{r} + aN\mathbf{n}), \tag{4}$$

where $\mathbf{n}$ runs over all vectors with all components integer and ρ is assumed to be defined as zero outside its original cell of definition. The potential obtained from it in the way outlined above is then periodic, too:

$$\phi_{\text{per}}(\mathbf{r}) = \sum_{\mathbf{n}} \phi(\mathbf{r} + aN\mathbf{n}). \tag{5}$$

This is the essential meaning of periodic boundary conditions. The problem is that ϕ, the exact potential of the isolated ρ, does not vanish outside the cell where ρ was defined, and our task is now to isolate the single contribution with $\mathbf{n} = 0$ from Eq. (5).

To do this, we note that we are interested in ϕ only inside the original cell, close to its "own" charge distribution ρ, whereas all the periodic repetitions of ρ are outside this cell at a larger distance. So it seems possible to describe them by the leading terms in their multipole expansion. Let ϕ' denote the approximation to ϕ obtained by cutting off the multipole expansion of ϕ after some leading terms. Inside the original cell we should have

$$\phi(\mathbf{r} + aN\mathbf{n}) \simeq \phi'(r + aN\mathbf{n}), \qquad \mathbf{n} \neq 0 \tag{6}$$

and we will obtain a potential with the influence of the repeated charge distribution subtracted approximately, by calculating

$$\phi_{\text{corr}}(\mathbf{r}) = \phi_{\text{per}}(\mathbf{r}) - \sum_{\mathbf{n}\neq 0} \phi'(\mathbf{r} + aN\mathbf{n}) \tag{7}$$

with $\mathbf{r}$ inside the original cell, or

$$\phi(\mathbf{r}) \simeq \phi_{\text{corr}}(\mathbf{r}) = \phi_{\text{per}}(\mathbf{r}) + \phi'(\mathbf{r}) - \sum_{\mathbf{n}} \phi'(\mathbf{r} + aN\mathbf{n}). \tag{8}$$

The advantage of the last formulation is that the sum on the right-hand side now is a completely periodic potential which may be calculated by the Fourier method from a multipole approximation ρ' to ρ, whereas $\phi'(\mathbf{r})$ inside the original cell is the exact field of ρ', which is well known and easily calculated for the first few multipoles.

Noting that the first and last terms on the right-hand side together constitute the field of a periodic array of charge distributions formed from $\rho - \rho'$, we can state the essence of the correction method as follows:

Step 1. Subtract a multipole approximation ρ' from the charge distribution ρ.

Step 2. Solve Poisson's equation for $\rho - \rho'$ to obtain the periodic field $E_{\text{per}} - E'_{\text{per}}$.

Step 3. Add the exact field generated by ρ' in the cell at the origin.

The accuracy of this method depends essentially on two approximations. The first one is the neglection of the periodicity of $E_{\text{per}} - E'_{\text{per}}$, which was justified by the essentially short-range behavior of this field, depending on the accuracy of the multipole expansion. The second one is the replacement of the sum in Eq. (8) by the Fourier solution to the Poisson equation. This may be serious, because a large discrepancy between this solution and the exact one may introduce an additional error into Eq. (5) (not counting the difference due to the different boundary conditions).

In the following we shall demonstrate the size of these errors with test calculations, and we shall show that the monopole approximation already yields a significant improvement in accuracy, but that the monopole has to be represented by a sufficiently "smooth" charge distribution. The calculations were done only for $\alpha = 0$, i.e., for Coulomb-type fields, but the results are easily generalizable to Yukawa fields. Because of the shorter range and exponential decay of the latter corrections should be of less importance for them.

The calculations were carried out on a $32 \times 32 \times 32$ mesh, and for simplicity, we used the complex Fourier transform. Also, to compare the more important physical quantities, we computed the fields directly, and not the potentials.

When selecting an appropriate charge distribution of pure monopole character, we first tried a point charge. However, it was found that in this case the field obtained by Fourier transform methods differed considerably from the exact field even at the center of the region, because a point charge cannot be represented adequately with a finite Fourier series. We therefore chose the following spherical charge distribution around the point $\mathbf{r}_0$:

$$\rho'(\mathbf{r}) = \frac{a^3}{\pi(\pi)^{1/2}} \exp(-a^2 r'^2), \qquad r' = |\mathbf{r} - \mathbf{r}_0| \tag{9}$$

the field of which is

$$\mathbf{E}(\mathbf{r}) = \frac{\mathbf{r} - \mathbf{r}_0}{13^{1/2}} [\operatorname{erf}(a \cdot r') - 2ar' \exp(-a^2 r'^2)(\pi)^{1/2}] \tag{10}$$

ρ' is normalized to a total charge of unity. To test the effectiveness of the method, the calculation was done for a charge distribution ρ, which cannot be represented well by a monopole but has known fields, namely a superposition of two distributions according to Eq. (9) at opposing positions $\mathbf{r}_0 = (-6, 0, 0)$ and $(+6, 0, 0)$

in the cube. The parameter a was chosen equal to 0.3. The resulting distribution is plotted along the x-axis in Fig. 1, together with the correcting monopole of the same functional shape, but located at the center.

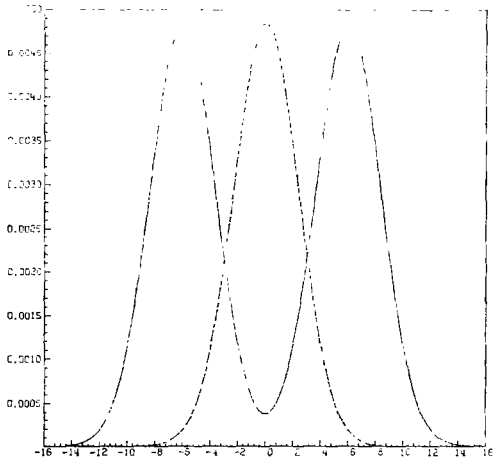

FIG. 1. Charge distribution used for the test calculations (full curve) and correcting monopole charge distribution (dashed curve).

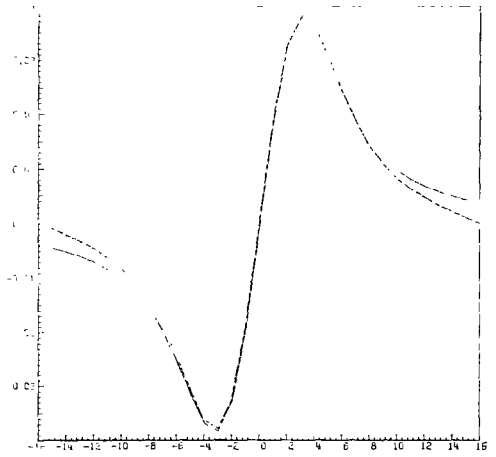

FIG. 2. Dashed curve, field of the periodically repeated monopole charge distribution of Fig. 1, calculated by the Fourier transform method. Full curve, exact field of the same distribution. The two fields differ near the boundary, but seem sufficiently equal near the center. Both curves were plotted with the number of discrete points used for the transform (i.e., 32).

Figure 2 shows the exact and the Fourier-obtained field of the monopole distribution (9). It can be seen that except for the necessary difference at the boundary, the Fourier solution appears sufficiently accurate.

In Fig. 3, the corrected and uncorrected fields obtained from the Fourier method are presented, together with the exact field for the two-monopole system. Apparently, the correction improves the result drastically in the range from about $x = 6$ to $x = 12$. The range of 5% accuracy of the solution is extended from $(-7, +7)$ to $(-12, +12)$, and even outside that the field may be sufficiently accurate for some purposes. Since the charge distribution in this case was practically confined to the $(-12, +12)$ range, we conclude that the actually used portion of space is now about 42% of the cell, whereas in the empty-cell method only 12.5% are used.

To get an idea of the magnitude of error throughout space, we show contour maps of the relative error

$$| \mathbf{E} - \mathbf{E}_{\text{exact}} | / | \mathbf{E}_{\text{exact}} | \qquad [\%]$$

in five different x–y planes located at $z = 0, 4, 8, 12, 16$, in Figs. 4–8. It should be noted that this definition of the error also takes into account directional deviations.

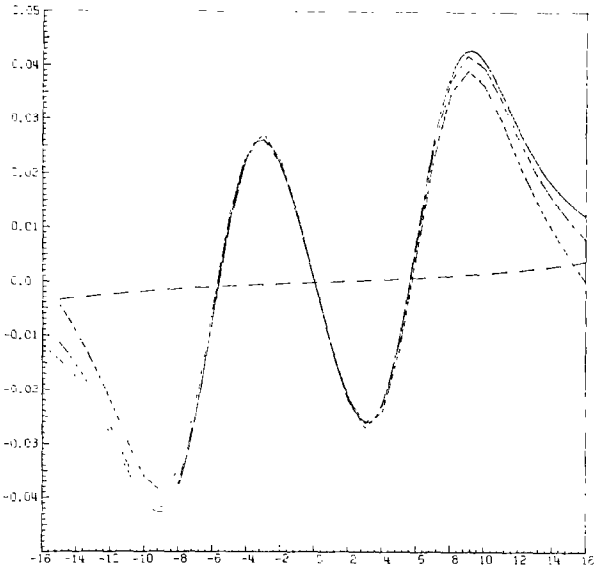

FIG. 3. Full curve, exact field of the two-monopole distribution of Fig. 1. Dash-dotted, Fourier solution with periodic behavior. Short dashes, correction to the field with the method discussed in this paper. Long dashes, final corrected field showing marked improvement towards the boundary.

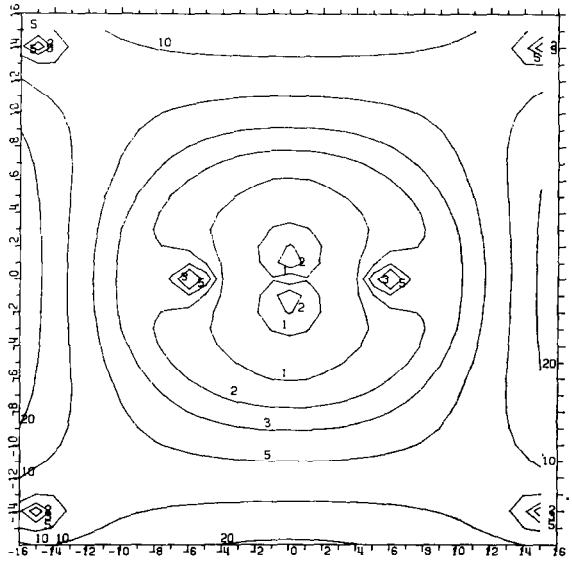

FIG. 4. Contour map of the relative error (%) in the field for the situation of Fig. 3 with the charges aligned along the x-axis. The error is plotted in the x–y plane at $z = 0$.

Apparently the behavior observed in the $z = 0$ plane along the x-axis holds true throughout space, in fact it is even better off this plane because the charge comes closest to the boundary on this plane.

Thus, even the simple monopole correction yields a significant improvement in accuracy. The computing time for evaluating the three field components on $32 \times 32 \times 32$ mesh points was 2 sec on an IBM-360/91.

If, however, aside from the gain in space, computation times are important, too, the calculation of the exact field according to Eq. (10) may be too involved. This can be avoided, if the total charge of the system is kept fixed and its center remains at the same position, which should hold for all dynamical systems with a fixed charge density over mass density ratio. Then the exact monopole field can be computed once and stored on tape.

It should be noted that although we have tested only fields in this discussion, because they are the physically most important quantity, the correction may to some advantage be done on the potential and the field components may then be obtained by numeric differentiation, so that only one correction is necessary.

Finally, we have presented the method in its simplest, straightforward application. It is clear to see that only minor modifications are needed to use it in two-dimensional calculations, and if a mixed Fourier-algebraic method is used with Fourier analysis in only one dimension, the correction may be used in this one

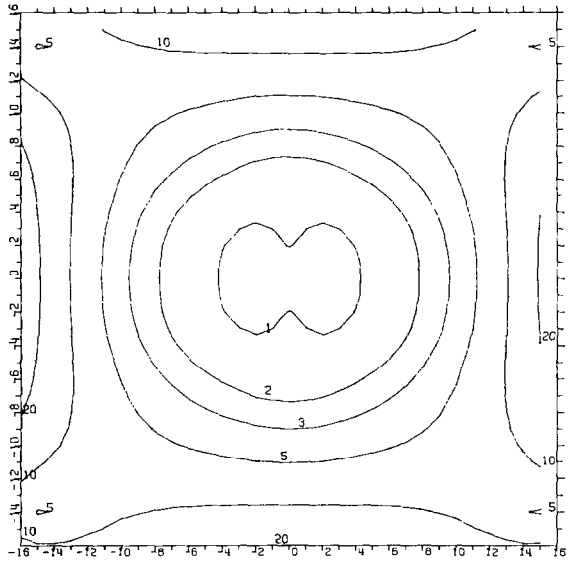

FIG. 5. Contour map of the relative error (%) in the field for the situation of Fig. 3 with the charges aligned along the x-axis. The error is plotted in the x–y plane at $z = 4$.

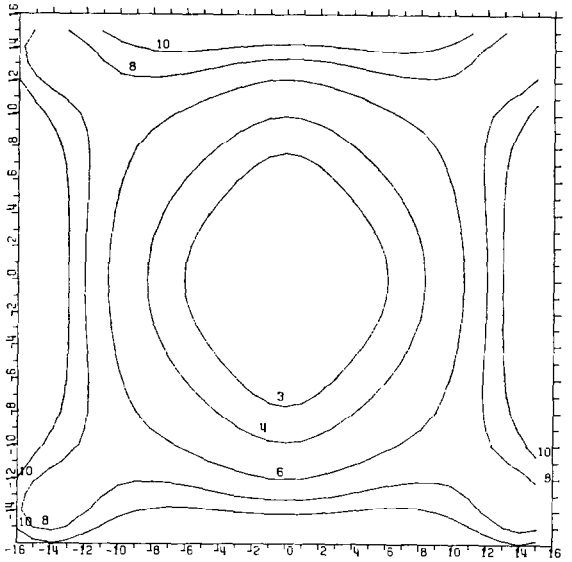

FIG. 6. Contour map of the relative error (%) in the field for the situation of Fig. 3 with the charges aligned along the x-axis. The error is plotted in the x–y plane at $z = 8$.

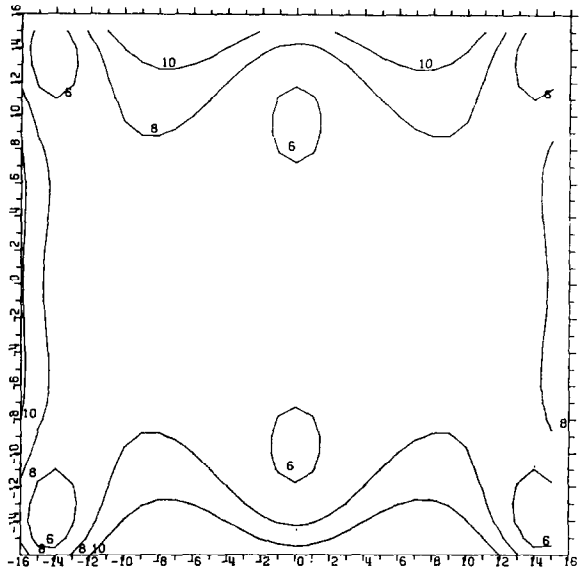

FIG. 7. Contour map of the relative error (%) in the field for the situation of Fig. 3 with the charges aligned along the x-axis. The error is plotted in the x–y plane at $z = 12$.

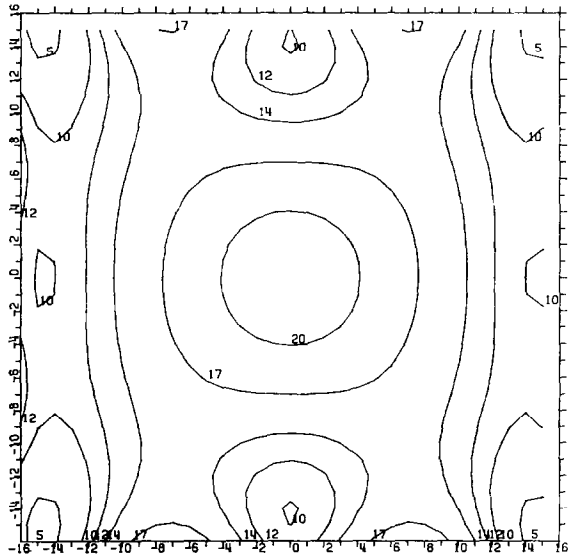

FIG. 8. Contour map of the relative error (%) in the field for the situation of Fig. 3 with the charges aligned along the x-axis. The error is plotted in the x–y plane at $z = 16$.

dimension. Furthermore, an even higher accuracy may be obtained by including higher-order multipoles in the expansion (this requires finding "smooth" charge distributions of the given multipolarity) or, on the other hand, using a different approximating charge distribution of arbitrary type with known field. The only requirement this has to fulfill is that it should reproduce the long-range behavior of the field.

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