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Fourth-Order Poisson Solver for the Simulation of Bounded Plasmas

G. KNORR, G. JOYCE, AND A. J. MARCUS

Department of Physics and Astronomy, The University of Iowa, Iowa City, Iowa 52242

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The solution of the two-dimensional Poisson equation in a rectangle with periodic boundaries in one direction and Dirichlet or Neumann boundaries in the other can be handled by a Fast Fourier Transform in one dimension and a fast nonperiodic procedure such as splines in the other. Such a solution is necessary for the simulation of semiperiodic plasma systems. A method is presented which is direct and of fourth order in *both* the electric potential and the electric fields.

1. INTRODUCTION

One of the components of any two-dimensional electrostatic particle simulation on a rectangular grid is the solution of Poisson's equation

$$\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}\right)\varphi(x, y)=\rho(x, y). \tag{1}$$

A class of numerical simulations requires periodic boundary conditions in one direction and either Dirichlet or Neumann boundary conditions in the other direction. For these problems we need *both* the potential and the electric fields, which we define for simplicity as

$$\mathbf{E}(x, y)=\nabla\varphi(x, y). \tag{2}$$

A large volume of literature exists on the solution of Poisson's equation to fourth- and higher-order accuracy and with various boundary conditions [1–8]. Little effort has been devoted, however, to the solution for which *both* the potential and the fields are obtained to high accuracy *and* for which the boundary conditions of our interest are easily implemented. We have found a direct scheme for solving Poisson's equation from which the potential and the fields can be obtained to fourth-order accuracy. The scheme is easily implemented and requires only Fast Fourier Transforms [9] which are available on any modern computer. The method uses spline techniques and is unusual only in the introduction of the integrated spline, which turns out to be optimal for the representation of second derivatives.

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In Section 2 we discuss a one-dimensional problem which will illustrate the technique. The method is applied to the two-dimensional Poisson equation in Section 3. Section 4 displays an example. Section 5 is the conclusion.

2. The One-Dimensional Poisson Equation

Most of the features of the method for solving the two-dimensional Poisson equation can be easily illustrated by investigating the numerical solution of the one-dimensional Poisson equation. We concentrate on the one-dimensional problem, since it is less cluttered. The extension to two dimensions is then simple to implement.

We consider cubic splines [10] interpolating a set of equidistant points $\tilde{E}_j$, $j = 0, 1, 2,..., n$, where $\tilde{E}(x)$ is the one-dimensional electric field. Let the distance between the points be Δx and the first and second derivatives in the knots be p_j and s_j, respectively. For $x_j < x < x_{j+1}$ we write

$$\tilde{E}(x) = \tilde{E}_j + p_j(x - x_j) + \tfrac{1}{2}s_j(x - x_j)^2 + g_j(x - x_j)^3, \tag{3}$$

where g_j is a constant which can be eliminated by the spline conditions. Applying the continuity conditions for splines, we find the following equations for the first and second derivatives:

$$\frac{1}{6}(p_{j+1} + 4p_j + p_{j-1}) = \frac{1}{2\Delta x}(\tilde{E}_{j+1} - \tilde{E}_{j-1}) \tag{4}$$

and

$$\frac{1}{6}(s_{j+1} + 4s_j + s_{j-1}) = \frac{1}{(\Delta x)^2}(\tilde{E}_{j+1} - 2\tilde{E}_j + \tilde{E}_{j-1}). \tag{5}$$

A standard Fourier mode analysis implemented by assuming

$$\tilde{E}_j = \tilde{E}\exp(i\kappa j), \qquad \rho_j = \rho\exp(i\kappa j), \qquad \kappa = k\,\Delta x \tag{6}$$

leads to

$$\rho = \frac{i\kappa}{\Delta x}\tilde{E}W_\rho(\kappa), \tag{7}$$

where

$$\tilde{W}_\rho(\kappa) = 3\sin\kappa/[\kappa(2 + \cos\kappa)]. \tag{8}$$

Note that $(i\kappa/\Delta x)\tilde{E}$ is the exact derivative of E, and $\tilde{W}_\rho(\kappa)$ is a filter function. For small κ we see that

$$\tilde{W}_\rho(\kappa) = 1 - \kappa^4/180 + \cdots$$

and for $\kappa = \pi/2$, and π,

$$\tilde{W}_\rho(\kappa = \pi/2) = 3/4 = 1 - 0.045, \qquad W_\rho(\kappa = \pi) = 0. \tag{10}$$

The value $\kappa = \pi$ corresponds to the "Nyquist wavelength" which is equal to two mesh widths. The long wavelengths are quite well represented up to half the Nyquist wavelength, whereas the shorter wavelength are heavily damped. This is a favorable filter characteristic, if we compute the ρ from the given $\tilde{E}_j$, because it damps short wavelength noise. It is ill suited, however, if E is the unknown quantity. According to Eq. (7), $\tilde{E}$ becomes singular due to the zero of $W_\rho(\kappa)$ at $\kappa = \pi$.

Looking at the second derivative, Eq (5), in the same way is disappointing. The lowest order appriximation to the right-hand side of Eq. (5) is not improved. Using the same method as before, we find

$$s = -\frac{\kappa^2 \tilde{E}}{(\Delta x)^2} W_s(\kappa), \tag{11}$$

where

$$W_s(\kappa) = \frac{6(1 - \cos\kappa)}{\kappa^2(2 + \cos\kappa)}. \tag{12}$$

For small κ

$$W_s(\kappa) = 1 + \kappa^2/12 + \cdots \tag{13}$$

and for $\kappa = \pi/2$

$$W_s(\kappa) = 12/\pi^2 = 1.216. \tag{14}$$

The filter $W_s(\kappa)$ is greater than one, which is good for integration purposes, but the scheme is of second order only. The use of a spline to solve a second-order differential equation is thus hardly justified.

A method which does yield fourth-order accuracy can be obtained by integrating Eq. (3) and making use of the continuity of the spline and its derivative. Let

$$\begin{aligned}\varphi_{j-1} - \varphi_j &= \int_{x_j}^{x_{j+1}} E(x')\,dx' \\ &= \frac{\Delta x}{2}(\tilde{E}_j + \tilde{E}_{j+1}) - \frac{(\Delta x)^2}{12}(\rho_{j+1} - \rho_j).\end{aligned} \tag{15}$$

Writing down the same formula with j decreased by one and subtracting gives

$$\varphi_{j+1} - 2\varphi_j + \varphi_{j-1} = \frac{\Delta x}{2}(\tilde{E}_{j+1} - \tilde{E}_{j-1}) - \frac{(\Delta x)^2}{12}(\rho_{j+1} - 2\rho_j + 2_{j-1}). \tag{16}$$

We eliminate $\tilde{E}_j$ using Eq. (4) and obtain

$$\varphi_{j+1} - 2\varphi_j + \varphi_{j-1} = \frac{(\Delta x)^2}{12}(\rho_{j-1} + 10\rho_j + \rho_{j+1}). \tag{17}$$

A modal analysis of Eq. (17) gives

$$\rho = -\frac{\kappa^2 \varphi}{(\Delta x)^2} \tilde{W}_\varphi(\kappa), \tag{18}$$

where

$$\tilde{W}_\varphi(\kappa) = \frac{12(1-\cos\kappa)}{\kappa^2(5+\cos\kappa)}. \tag{19}$$

For small κ

$$\tilde{W}_\varphi = 1 - \kappa^4/240 + \cdots \tag{20}$$

and for shorter wavelengths

$$\tilde{W}_\varphi(\pi/2) = \frac{48}{5\pi^2} = 1 - 0.0273, \qquad W_\varphi(\pi) = \frac{6}{\pi^2} = 0.6. \tag{21}$$

Equation (17) represents a fourth-order scheme. The short wavelengths are exaggerated by up to a factor of $\pi^2/6$, rather than damped. Our principal interest, however, is the determination of the electric fields and we will see that if the fields are determined by fitting a spline through the φ's, the short wavelength field components will be damped. We note here that Eq. (17) is actually quite old and has been used as early as 1935 [11] and more recently by Adam [8]. Its relation to splines has not previously been reported. We have seen that if Eq. (4) is used to determine the electric field, the short wavelength components of $\tilde{E}$ are amplified. We, therefore, put a spline through the φ_j's and calculate E_j from

$$E_{j+1} + 4E_j + E_{j-1} = (3/\Delta x)(\varphi_{j+1} - \varphi_{j-1}), \qquad j = 2, \ldots, n-1. \tag{22}$$

The accuracy is obtained from mode analysis. We find

$$E = \rho \frac{\Delta x}{i\kappa} W_\rho(\kappa) \tag{23}$$

with

$$W_\rho(\kappa) = \tilde{W}_\rho(\kappa)/\tilde{W}_\varphi(\kappa). \tag{24}$$

For small κ

$$W_\rho(\kappa) = 1 - \kappa^4/720 + \cdots \tag{25}$$

and for short wavelengths,

$$W_\rho(\pi/2) = \frac{5\pi}{16} = 1 - 0.01825, \qquad W_\rho(\pi) = 0. \tag{26}$$

E is of fourth-order accuracy and the error coefficient is very small indeed. At half the Nyquist wavelength, the error is less than 2 %.

For Dirichlet boundary conditions we prescribe the values φ_1 and φ_n, the boundary values of the potential. In order to solve Eq. (22) we must supply E_1 and E_n. This appears paradoxical because once $\varphi(x)$ has been determined, its derivative should be known everywhere. This is, in fact, the case since from Eq. (15)

$$E_1 = \frac{2}{\Delta x}(\varphi_2 - \varphi_1) - E_2 + \frac{\Delta x}{6}(\rho_2 - \rho_1),$$

$$E_n = \frac{2}{\Delta x}(\varphi_n - \varphi_{n-1}) - E_{n-1} + \frac{\Delta x}{6}(\rho_n - \rho_{n-1}). \tag{27}$$

Neumann boundary conditions are more complicated. In order to find φ_1 and φ_n, we proceed as follows. A suitable combination of Eq. (15) and Eq. (22) gives

$$-2E_{j-1}\Delta x = \varphi_{j+1} - 4\varphi_j + 3\varphi_{j-1} + (\Delta x/6)(\rho_{j+1} - 2\rho_j + 3\rho_{j-1}),$$

where we have neglected the difference between E_j and $\tilde{E}_j$. When this is combined with Eq. (17), we obtain

$$\varphi_1 = \varphi_2 - E_1\Delta x + ((\Delta x)^2/24)(\rho_3 - 6\rho_2 - 7\rho_1) \tag{28}$$

and

$$\varphi_n = \varphi_{n-1} + E_n\Delta x + ((\Delta x)^2/24)(-7\rho_n - 6\rho_{n-1} + \rho_{n-2}). \tag{29}$$

Equations (17), (28) and (29) are now exactly n equations for the n unknowns φ_j, with E_1 and E_n prescribed.

The features of the one-dimensional spline fitting solution of the one-dimensional Poisson equation can be carried over to the two-dimensional case.

3. The Two-Dimensional Poisson Equation

We now consider the solution of Poisson's equation in two dimensions to fourth-order accuracy. We assume that in the x direction, the equation is periodic in an interval of length L_x. First we write

$$\varphi(x, y) = \sum_k \varphi_k(y)\, e^{ikx}, \qquad k = (2\pi/L_x)n,$$

$$\rho(x, y) = \textstyle\sum_k \rho_k(y)\, e^{ikx}. \tag{30}$$

It is advantageous to use x as the periodic variable because the x values are stored in a row in a FORTRAN program and are easily accessible to a FFT.

We insert Eq. (30) into Eq. (1), but introduce a form factor $a(\kappa)$ ($\kappa = k\,\Delta x$), in addition, which will be chosen for our convenience. Equation (1) becomes

$$\frac{\partial^2}{\partial y^2}\varphi_k(y) - k^2 a(\kappa)\,\varphi_k = \rho_k(y). \tag{31}$$

Equation (31) is discretized according to Eq. (17) as

$$\begin{aligned}&\frac{12}{(\Delta y)^2}(\varphi_{k,\mu+1} - 2\varphi_{k,\mu} + \varphi_{k,\mu-1})\\ &\quad = (\rho_{k,\mu-1} + 10\rho_{k,\mu} + \rho_{k,\mu-1}) + k^2 a(\kappa)(\varphi_{k,\mu-1} + 10\varphi_{k,\mu} + \varphi_{k,\mu+1}).\end{aligned} \tag{32}$$

We now introduce Fourier modes in the y direction,

$$\varphi_l(y) = \varphi \exp(ily); \qquad l = (2\pi/L_y)m, \qquad m = 0, 1, 2,..., \tag{33}$$

and a corresponding expression for the charge density. With $\lambda = l\,\Delta y$, $\kappa = k\,\Delta x$, the mode analysis can be written as

$$\varphi = -\rho\Big/\left[l^2\,\frac{12(1-\cos\lambda)}{\lambda^2(5+\cos\lambda)} + k^2 a(\kappa)\right]. \tag{34}$$

To make the scheme fourth order, we choose

$$a(\kappa) = \frac{12(1-\cos\kappa)}{\kappa^2(5+\cos\kappa)}, \tag{35}$$

which for small κ is

$$a(\kappa) = 1 - \kappa^4/240. \tag{36}$$

This choice of the form factor keeps the error term of fourth order and makes the Fourier modes symmetric in the x and y directions. There is still an overemphasis of the short wavelength terms of up to a fector $\pi^2/6$. We now write the tridiagonal system as

$$\begin{aligned}&(1-c_k)\,\varphi_{k,\mu+1} - (2+10c_k)\,\varphi_{k,\mu} + (1-c_k)\,\varphi_{k,\mu-1}\\ &\quad = \frac{1}{12}(\rho_{k,\mu+1} + 10\rho_{k,\mu} + \rho_{k,\mu-1}), \qquad \mu = 2 \cdots (n+1),\end{aligned} \tag{37}$$

with

$$c_k = k^2 a(\kappa)/12.$$

(The solution to Eq. (37) can be determined once the boundary conditions are applied.)

The boundary conditions must still be applied at the upper and lower boundaries. For Dirichlet boundary conditions $\varphi_{k,1}$, $\varphi_{k,n}$ are given and the solution of Eq. (37) is straightforward. For Neumann boundary conditions, Eq. (37) must be supplemented by a generalization of Eqs. (28) and (29).

$$\begin{aligned}-(1-c_k)(1+4c_k)\,\varphi_{k,1} &+ (1-3c_k+8c_k^2)\,\varphi_{k,2}\\ &= (1-c_k)\,E_{k,1}\,\Delta y - \frac{1-c_k}{12}(\rho_{k,3}+2\rho_{k,2}-3\rho_{k,1})\,\Delta y^2\\ &\quad + \frac{(1-2c_k)}{24}(\rho_{k,3}+10\rho_{k,2}+\rho_{k,1})\,\Delta y^2\end{aligned} \tag{38}$$

and

$$\begin{aligned}(1-c_k)(1+4c_k)\,\varphi_{k,n} &- (1-3c_k+8c_k^2)\,\varphi_{k,n-1}\\ &= (1-c_k)\,E_{k,n}\,\Delta y + \frac{1-c_k}{12}(\rho_{k,n-2}+2\rho_{k,n-1}-3\rho_{k,n})\,\Delta y^2\\ &\quad - \frac{1-2c_k}{24}(\rho_{k,n}+10\rho_{k,n-1}+\rho_{k,n-2})\,\Delta y^2.\end{aligned} \tag{39}$$

The right sides of Eqs. (38) and (39) are known quantities. Once the $\varphi_{k,\mu+1}$ have been calculated, we can proceed in two ways to obtain the fields:

(a) Obtain the $\tilde{E}^y_{k,\mu}$ from

$$\tilde{E}^y_{k,\mu+1} + 4\tilde{E}^y_{k,\mu} + \tilde{E}^y_{k,\mu-1} = \frac{3}{\Delta y}(\varphi_{k,\mu-1} - \varphi_{k,\mu-1}), \qquad \mu = 2 \cdots (n-1), \tag{40}$$

which is supplemented by

$$\begin{aligned}E^y_{k,1} + E^y_{k,2} &= \frac{2}{\Delta y}(1+c_k)(\varphi_{k,2}-\varphi_{k,1}) + \frac{1}{6}(\rho_{k,2}-\rho_{k,1})\,\Delta y,\\ E^y_{k,n} + E^y_{k,n-1} &= \frac{2}{\Delta y}(1+c_k)(\varphi_{k,n}-\varphi_{k,n-1}) + \frac{1}{6}(\rho_{k,n}-\rho_{k,n-1})\,\Delta y.\end{aligned} \tag{41}$$

These equations are a generalization of Eq. (27). For the x components of the electric field, we write

$$\tilde{E}^x_{k,\mu} = ik\sigma(\kappa)\,\varphi_{k,\mu}, \tag{42}$$

where $\sigma(k)$ is determined below. From the known $\tilde{E}^x_{k,\mu}$ and $\tilde{E}^y_{k,\mu}$, we obtain $\tilde{E}^x_{v,\mu}$ and $\tilde{E}^y_{v,\mu}$, the components of the electric field in x–y space, by a FFT.

(b) We obtain $\varphi_{\nu,\mu}$ directly from $\varphi_{k,\mu}$ by a FFT. $E^{x}_{\nu,\mu}$ is calculated from

$$\tilde{E}^{x}_{\nu+1,\mu} + 4\tilde{E}^{x}_{\nu,\mu} + \tilde{E}^{x}_{\nu-1,\mu} = (3/\Delta x)(\varphi_{\nu-1,\mu} - \varphi_{\nu-1,\mu}) \tag{43}$$

using a periodic spline. $\tilde{E}^{y}_{\nu,\mu}$ is calculated from

$$\tilde{E}^{y}_{\nu,\mu+1} + 4\tilde{E}^{y}_{\nu,\mu} + \tilde{E}^{x}_{\nu-1,\mu} = (3/\Delta x)(\varphi_{\nu,\varphi+1} - \varphi_{\nu,\mu-1}). \tag{44}$$

This equation has to be supplemented by the Fourier transform of Eq. (41). Both methods appear to require about the same computer time. The form factor $\sigma(\kappa)$ in (42) is determined by comparing (42) with (43). With a mode analysis, we immediately find

$$\sigma(\kappa) = \frac{3 \sin \kappa}{\kappa(2 + \cos \kappa)}. \tag{45}$$

4. An Example

In order to check the accuracy of the method, we have written a computer program to solve the equation

$$\frac{\partial^2 \varphi}{\partial x^2} + \frac{\partial^2 \varphi}{\partial y^2} = \sin[(2\pi/8)\, k_x x] \cdot \sin[(2\pi/8)\, k_y y] \tag{46}$$

subject to the boundary conditions $\varphi(x, y = 0) = \varphi(x, y = 16) = 0$ and periodic boundaries for $x = 0$ and $x = 16$. k_x and k_y are integers. The exact solution

$$\varphi = -\left[\left(\frac{2\pi}{8}\right)^2 (k_x^2 + k_y^2)\right]^{-1} \sin\left(\frac{2\pi}{8} k_x x\right) \sin\left(\frac{2\pi}{8} k_y y\right) \tag{47}$$

contains only a single mode, and provides a simple test of the estimated accuracy of the algorithm. From Eq. (20), we expect the relative error to vary as $k^4 = (k_x^2 + k_y^2)^2$ for values of k_x and k_y chosen for the right-hand side of (46). The equation was solved on a 16×16 mesh with $\Delta x = \Delta y = 1$. Table I is a record for various runs of the average relative deviations, for example, $\Delta\varphi_{A\nu} = (1/n) \sum_{\nu=1}^{n} |\Delta\varphi_\nu|$. Boundary points and mesh points at which the exact function was zero were excluded. Only values of k_x and k_y were changed from run to run. We normalized the relative error of the runs by dividing by k^4. It is seen that the normalized errors in the table are approximately the same. This is expected in a fourth-order method. The table contains a few "mirror" cases, for example, (k_x, k_y) equal to (1, 3) and (3, 1). The exact solutions are mirror images of each other. This symmetry is reflected in the table: The average errors for the potentials are the same and the errors for the electric fields exhibit approximately the same symmetry. The agreement is not perfect however, because of rounding errors, and the use of periodic and nonperiodic splines.

TABLE I

k_x, k_y	$\Delta\varphi_{Av}$	$\frac{\Delta\varphi_{Av}}{k^4}$	ΔE_{xAv}	ΔE_{yAv}	$\frac{\Delta E_{xAv}}{k^4}$	$\frac{\Delta E_{yAv}}{k^4}$
1,1	9.95×10^{-5}	2.48×10^{-5}	3.35×10^{-5}	3.47×10^{-5}	8.38×10^{-6}	8.68×10^{-6}
1,2	1.32×10^{-3}	5.28×10^{-5}	1.18×10^{-3}	9.22×10^{-4}	4.72×10^{-5}	3.69×10^{-5}
1,3	7.64×10^{-3}	7.64×10^{-5}	7.51×10^{-3}	5.55×10^{-3}	7.51×10^{-5}	5.55×10^{-5}
2,1	1.32×10^{-3}	5.28×10^{-5}	9.59×10^{-4}	1.19×10^{-3}	3.84×10^{-5}	4.76×10^{-5}
2,2	1.62×10^{-3}	2.53×10^{-5}	6.55×10^{-4}	6.19×10^{-4}	1.02×10^{-5}	9.69×10^{-6}
2,3	6.37×10^{-3}	3.77×10^{-5}	4.07×10^{-3}	6.80×10^{-3}	2.41×10^{-5}	4.02×10^{-5}
3,1	7.64×10^{-3}	7.64×10^{-5}	5.06×10^{-3}	7.51×10^{-3}	5.06×10^{-5}	7.51×10^{-5}
3,2	6.36×10^{-3}	3.76×10^{-5}	6.32×10^{-3}	4.11×10^{-3}	3.74×10^{-5}	2.43×10^{-5}
3,3	8.49×10^{-3}	2.62×10^{-5}	4.22×10^{-3}	4.70×10^{-3}	1.30×10^{-5}	1.45×10^{-5}
4,1	2.64×10^{-2}	9.13×10^{-5}	1.98×10^{-2}	2.62×10^{-2}	6.85×10^{-5}	9.06×10^{-5}
4,2	2.26×10^{-2}	5.65×10^{-5}	2.34×10^{-2}	2.04×10^{-2}	5.85×10^{-5}	5.10×10^{-5}
4,3	2.09×10^{-2}	3.34×10^{-5}	2.51×10^{-2}	7.58×10^{-3}	4.00×10^{-5}	1.21×10^{-5}

The accuracy obtained, even for wavelengths as short as twice the Nyquist wavelength, is quite satisfactory.

5. Conclusion

We have presented a method which can be used to provide solutions to Poisson's equation in simulating bounded plasma systems. The method is direct and moderately fast and provides fourth-order accuracy to *both* the electric potential and the electric fields. In addition, it is easily implemented since only Fast Fourier Transforms and tridiagonal matrix inversions are used. A number of computer simulations of bounded plasma systems have recently appeared [12, 13] and this method may be useful in further investigations.

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