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Direct Numerical Solution of Poisson's Equation in Cylindrical (r, z) Coordinates

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Abstract

A direct solver method is developed for solving Poisson's equation numerically for the electrostatic potential $\phi(r, z)$ in a cylindrical region $(r < R_{wall},\ 0 < z < L)$. The method assumes the charge density $\rho(r, z)$ and wall potential $\phi(r = R_{wall}, z)$ are specified, and $\partial\phi/\partial z = 0$ at the axial boundaries $(z = 0, L)$.

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Many calculations in plasma physics require a rapid solution of Poisson's equation

$$\nabla^2 \phi = -4\pi\rho, \tag{1}$$

where ϕ is the electrostatic potential, and ρ is the charge density. This paper was motivated by the need to determine the potential variation in an axisymmetric Malmberg-Penning trap confining a pure electron plasma [1–3]. Hughes [4] has previously described a direct solver for Poisson's equation in cylindrical (r, z) coordinates, but the potentials on axis $(r = 0)$ and at some radius $r = r_0$ must be known. Often, the axial potential is not known *a priori.* Trunec [5] has also developed a direct Poisson solver in cylindrically symmetric geometry *without* requiring knowledge of the axial potential. Both Hughes and Trunec utilize a Fourier transform in the axial direction, but Trunec approximates the radial solution using the basis functions for cubic splines, while Hughes finds a radial solution using only the finite-difference form of the radial differential equation. Trunec's approach allows for unequal grid spacing in the radial direction, but the benchmarking results suggest that the spline approximation introduces more error than Hughes' method of solving the finite-difference equations directly. The purpose of this Note is to extend Hughes' solver so that it does not require knowledge of the axial potential.

For $\partial/\partial\theta = 0$, Poisson's equation in cylindrical (r, z) coordinates is

$$\frac{\partial^2 \phi}{\partial r^2} + \frac{1}{r}\frac{\partial \phi}{\partial r} + \frac{\partial^2 \phi}{\partial z^2} = -4\pi\rho, \tag{2}$$

where ϕ is the electrostatic potential, and ρ is the known charge density. The potential is assumed to be specified at radius $r = R_{wall}$, and $\partial\phi/\partial z = 0$ at the axial boundaries $(z = 0, L)$. The latter assumption is appropriate for the applications of interest, but can easily be modified to describe the case where $\phi = 0$ at the axial boundaries or the case of periodic boundary conditions by using a sine or Fourier transform instead of a cosine transform.

We begin the analysis by applying a discrete cosine transform in the axial ($\hat{z}$) direction to Poisson's equation. The cosine transform uses cosines only to form a complete set of basis functions in the interval from 0 to 2π, and guarantees that the solution will have zero derivative at the axial boundaries [6]. The cosine transform is defined by

$$F_k = \sum_{j=0}^{N-1} f_j \cos\frac{\pi k(j+\frac{1}{2})}{N}, \tag{3}$$

with inverse

$$f_j = \frac{2}{N}\sum_{k=0}^{N-1}{}' F_k \cos\frac{\pi k(j+\frac{1}{2})}{N}. \tag{4}$$

Here, the prime on the summation symbol means that the $k = 0$ term has a coefficient of $\frac{1}{2}$ multiplying $(2/N)F_0$.

We consider the (r, z) plane covered by a uniform mesh with constant spacing Δ_r and Δ_z in the r and z directions:

$$\begin{aligned} z &= (i+\frac{1}{2})\cdot\Delta_z, \quad i = 0,\ 1, ..., N_Z - 1, \\ r &= j\cdot\Delta_r, \quad j = 0,\ 1, ..., N_R, \end{aligned} \tag{5}$$

where $\Delta_z = \frac{L}{N_Z}$ and $\Delta_r = \frac{R_{wall}}{N_R}$. The cosine transform can be written as

$$\phi(r,z) = \frac{2}{N_Z} \sum_{k=0}^{N_Z-1}{}' \tilde{\phi}_k(r) \cos \frac{\pi k z}{\Delta_z N_Z}. \tag{6}$$

Substituting Eq. (6) into Poisson's equation (2) yields

$$\frac{\partial^2 \tilde{\phi}_k}{\partial r^2} + \frac{1}{r}\frac{\partial \tilde{\phi}_k}{\partial r} - \frac{1}{\Delta_z^2}\left(\frac{\pi k}{N_Z}\right)^2 \tilde{\phi}_k = -4\pi \tilde{\rho}_k. \tag{7}$$

where ρ has been similarly transformed.

The next step is to write these equations in finite-difference form. Away from the axis ($j \geq 1$), Eq. (7) becomes

$$\begin{aligned} \frac{\tilde{\phi}_{k,j+1} - 2\tilde{\phi}_{k,j} + \tilde{\phi}_{k,j-1}}{\Delta_r^2} &+ \frac{\tilde{\phi}_{k,j+1} - \tilde{\phi}_{k,j-1}}{2j\Delta_r^2} \\ -\frac{1}{\Delta_z^2}\left(\frac{\pi k}{N_Z}\right)^2 \tilde{\phi}_{k,j} &= -4\pi\tilde{\rho}_{k,j} \qquad (j \geq 1). \end{aligned} \tag{8}$$

Collecting terms yields

$$\tilde{\phi}_{k,j}\left[2 + \frac{\Delta_r^2}{\Delta_z^2}\left(\frac{\pi k}{N_Z}\right)^2\right] - \tilde{\phi}_{k,j-1}\left(1 - \frac{1}{2j}\right) - \tilde{\phi}_{k,j+1}\left(1 + \frac{1}{2j}\right) = 4\pi\Delta_r^2\tilde{\rho}_{k,j}. \tag{9}$$

Defining

$$
\begin{aligned}
S_{k,j} &= 4\pi\Delta_r^2\tilde{\rho}_{k,j}, \\
\lambda_k &= 2+\frac{\Delta_r^2}{\Delta_z^2}\left(\frac{\pi k}{N_Z}\right)^2, \\
\beta_j &= 1+\frac{1}{2j}, \\
\gamma_j &= 1-\frac{1}{2j},
\end{aligned}
\tag{10}
$$

we can rewrite Eq. (9) as

$$
-\gamma_j\tilde{\phi}_{k,j-1}+\lambda_k\tilde{\phi}_{k,j}-\beta_j\tilde{\phi}_{k,j+1}=S_{k,j}. \tag{11}
$$

Equation (11) corresponds to the set of equations

$$
\begin{bmatrix}
-\gamma_1 & \lambda_k & -\beta_1 & 0 & \cdots & & & \\
0 & -\gamma_2 & \lambda_k & -\beta_2 & \cdots & & & \\
 & & & & \cdots & & & \\
 & & & & \cdots & -\gamma_{N_R-1} & \lambda_k & -\beta_{N_R-1}
\end{bmatrix}
\cdot
\begin{bmatrix}
\tilde{\phi}_{k,0} \\ \tilde{\phi}_{k,1} \\ \vdots \\ \tilde{\phi}_{k,N_R-1} \\ \tilde{\phi}_{k,N_R}
\end{bmatrix}
=
\begin{bmatrix}
S_{k,1} \\ S_{k,2} \\ \vdots \\ S_{k,N_R-1}
\end{bmatrix}
\tag{12}
$$

where it appears that there are N_R-1 equations and N_R+1 unknowns. However, we have assumed that the potential is specified at the radial boundary so that $\tilde{\phi}_{k,N_R}$ is known. The set of equations is then

$$\begin{bmatrix} -\gamma_1 & \lambda_k & -\beta_1 & 0 & \cdots & & & \\ 0 & -\gamma_2 & \lambda_k & -\beta_2 & \cdots & & & \\ & & & & \cdots & & & \\ & & & & \cdots & -\gamma_{N_R-2} & \lambda_k & -\beta_{N_R-2} \\ & & & & \cdots & 0 & -\gamma_{N_R-1} & \lambda_k \end{bmatrix} \cdot \begin{bmatrix} \tilde{\phi}_{k,0} \\ \tilde{\phi}_{k,1} \\ \vdots \\ \tilde{\phi}_{k,N_R-1} \end{bmatrix}$$

$$= \begin{bmatrix} S_{k,1} \\ S_{k,2} \\ \vdots \\ S_{k,N_R-1} + \beta_{N_R-1}\tilde{\phi}_{k,N_R} \end{bmatrix} \quad (13)$$

We could similarly assume that the potential on axis, $\tilde{\phi}_{k,0}$, is specified and we would have a set of $N_R - 1$ equations and $N_R - 1$ unknowns.

Instead, we will find an additional equation utilizing the symmetry on axis. To proceed, a finite-difference form of Poisson's equation is required that is valid for $j = 0$. To find such an expression, we take the limit of Eq. (7) (the cosine-transformed Poisson's equation in differential form) as $r \to 0$, i.e.,

$$\lim_{r\to 0}\left\{\frac{\partial^2\tilde{\phi}_k}{\partial r^2} + \frac{1}{r}\frac{\partial\tilde{\phi}_k}{\partial r} - \frac{1}{\Delta_z^2}\left(\frac{\pi k}{N_Z}\right)^2\tilde{\phi}_k = -4\pi\tilde{\rho}_k\right\}. \quad (14)$$

The second term can be expressed differently in this limit. Using L'Hospital's rule, we find

$$\lim_{r\to 0} \frac{\frac{\partial \phi}{\partial r}}{r} = \frac{\partial^2 \phi}{\partial r^2}. \tag{15}$$

Thus, in the limit as $r \to 0$, the cosine-transformed Poisson's equation becomes

$$2\frac{\partial^2 \tilde{\phi}_k}{\partial r^2} - \frac{1}{\Delta_z^2}\left(\frac{\pi k}{N_Z}\right)^2 \tilde{\phi}_k = -4\pi\tilde{\rho}_k. \tag{16}$$

The finite-difference form of Eq. (16) is

$$2\frac{\tilde{\phi}_{k,+1} - 2\tilde{\phi}_{k,0} + \tilde{\phi}_{k,-1}}{\Delta_r^2} - \frac{1}{\Delta_z^2}\left(\frac{\pi k}{N_Z}\right)^2 \tilde{\phi}_{k,0} = -4\pi\tilde{\rho}_{k,0}, \tag{17}$$

where $j = 0$ has been substituted since we will use this equation only on axis. Next, utilizing the axial boundary condition $\partial\phi/\partial r|_{r=0} = 0$, we find that $\tilde{\phi}_{k,-1} = \tilde{\phi}_{k,+1}$. This result might have been anticipated simply by noting the assumed azimuthal symmetry in the problem. To show that the boundary condition also implies this result, recall that a three-point finite-difference approximation for a derivative is [7]

$$\left.\frac{\partial f}{\partial x}\right|_{x=x_0} = \frac{1}{2\Delta}[f(x_0 + \Delta) - f(x_0 - \Delta)]. \tag{18}$$

The finite difference form for the axial boundary conditions used here is therefore

$$\left.\frac{\partial \tilde{\phi}_k}{\partial r}\right|_{r=0} = [\tilde{\phi}_{k,+1} - \tilde{\phi}_{k,-1}]/(2\Delta_r) = 0,$$

or

$$\tilde{\phi}_{k,+1} = \tilde{\phi}_{k,-1}. \tag{19}$$

Substituting Eq. (19) into Eq. (17) yields

$$4\frac{\tilde{\phi}_{k,+1} - \tilde{\phi}_{k,0}}{\Delta_r^2} - \frac{1}{\Delta_z^2}\left(\frac{\pi k}{N_Z}\right)^2 \tilde{\phi}_{k,0} = -4\pi\tilde{\rho}_{k,0} \ ,$$

which can be expressed as

$$(2+\lambda_k)\tilde{\phi}_{k,0} - 4\tilde{\phi}_{k,1} = S_{k,0}. \tag{20}$$

The complete set of equations then becomes

$$\begin{bmatrix} 2+\lambda_k & -4 & 0 & \cdots & & & \\ -\gamma_1 & \lambda_k & -\beta_1 & \cdots & & & \\ & & & \cdots & & & \\ & & & \cdots & -\gamma_{N_R-2} & \lambda_k & -\beta_{N_R-2} \\ & & & \cdots & 0 & -\gamma_{N_R-1} & \lambda_k \end{bmatrix} \cdot \begin{bmatrix} \tilde{\phi}_{k,0} \\ \tilde{\phi}_{k,1} \\ \vdots \\ \tilde{\phi}_{k,N_R-2} \\ \tilde{\phi}_{k,N_R-1} \end{bmatrix} = \begin{bmatrix} S_{k,0} \\ S_{k,1} \\ \vdots \\ S_{k,N_R-2} \\ S_{k,N_R-1} + \beta_{N_R-1}\tilde{\phi}_{k,N_R} \end{bmatrix} \tag{21}$$

This tridiagonal system of N_R equations in N_R unknowns can be quickly solved in $\mathcal{O}(N_R)$ operations and the solution can be encoded very concisely [6]. This process is repeated for each wavenumber k, and finally the inverse cosine transform is used to find the potential $\phi(r, z)$.

A Poisson solver based on Eq. (21) has been written and benchmarked against a few analytically solvable cases. The first case is that of constant charge density ρ from $r = 0$ to $r = R_{wall}(1 - \epsilon)$, $0 < \epsilon \ll 1$, and constant wall potential $\phi|_{R_{wall}}$ at $r = R_{wall}$. The analytic solution (in MKS units) is

$$\phi(r) = \phi|_{R_{wall}} + \frac{\rho}{4\epsilon_0}(R_{wall}^2 - r^2). \tag{22}$$

We choose the potential at the wall, $\phi|_{R_{wall}} = 0$, the charge density $\rho = 1\ Coulomb/m^3$, and the wall radius, $R_{wall} = 0.01\ m$. Substituting into Eq. (22) gives

$$\phi(r) = 2.824 \cdot 10^{10}(10^{-4} - r^2)\ \ Volts. \tag{23}$$

Figure 1 shows a plot of the potential calculated directly from Eq. (23) and a plot of the difference between the potential calculated using the Poisson solver and by using Eq. (23). Thirty-two radial grid points were used for the Poisson solver.

The second case is that of a vacuum potential (zero charge density) with a sinusoidal wall potential $V_0 \cos(2\pi z/L)$. The analytical solution to Poisson's equation is

$$\phi(r, z) = \frac{V_0}{I_0(2\pi R_{wall}/L)} \cos(2\pi z/L) I_0(2\pi r/L), \tag{24}$$

where $I_0(x)$ is the modified Bessel function of order zero. Figure 2(a) shows an $r-z$ plot of Eq. (24) with $V_0 = 1V$, $R_{wall} = 0.02\,m$ and $L = 0.08\,m$. Figure 2(b) shows the difference between the analytic solution and the solution found from the Poisson solver using 32 radial and 32 axial grid points.

The maximum error in the potential is found to decrease initially as the square of the number of radial grid points used. This is likely due to the error involved in the finite-difference approximation of the derivatives. The first and second derivatives both have errors that are dependent on the square of the grid spacing, i.e.,

$$\begin{aligned} f'(x_0) &= \frac{1}{2\Delta}[f(x_0+\Delta) - f(x_0-\Delta)] - \frac{\Delta^2}{6} f^{(3)}(\xi), \\ f''(x_0) &= \frac{1}{\Delta^2}[f(x_0-\Delta) - 2f(x_0) + f(x_0+\Delta)] - \frac{\Delta^2}{12} f^{(4)}(\xi), \end{aligned} \tag{25}$$

for some ξ in the interval $x_0 - \Delta < \xi < x_0 + \Delta$ [7]. However, the error in the potential eventually reaches a minimum and begins to increase with increasing number of grid points (decreasing grid spacing Δ) because of round-off error.

In conclusion, the direct solver developed here is a fast and straightforward approach to solving Poisson's equation in cylindrically symmetric geometry given only the potential variation at some radius, $\phi(r = R_{wall}, z)$, and the charge density distribution, $\rho(r, z)$.

Acknowledgements

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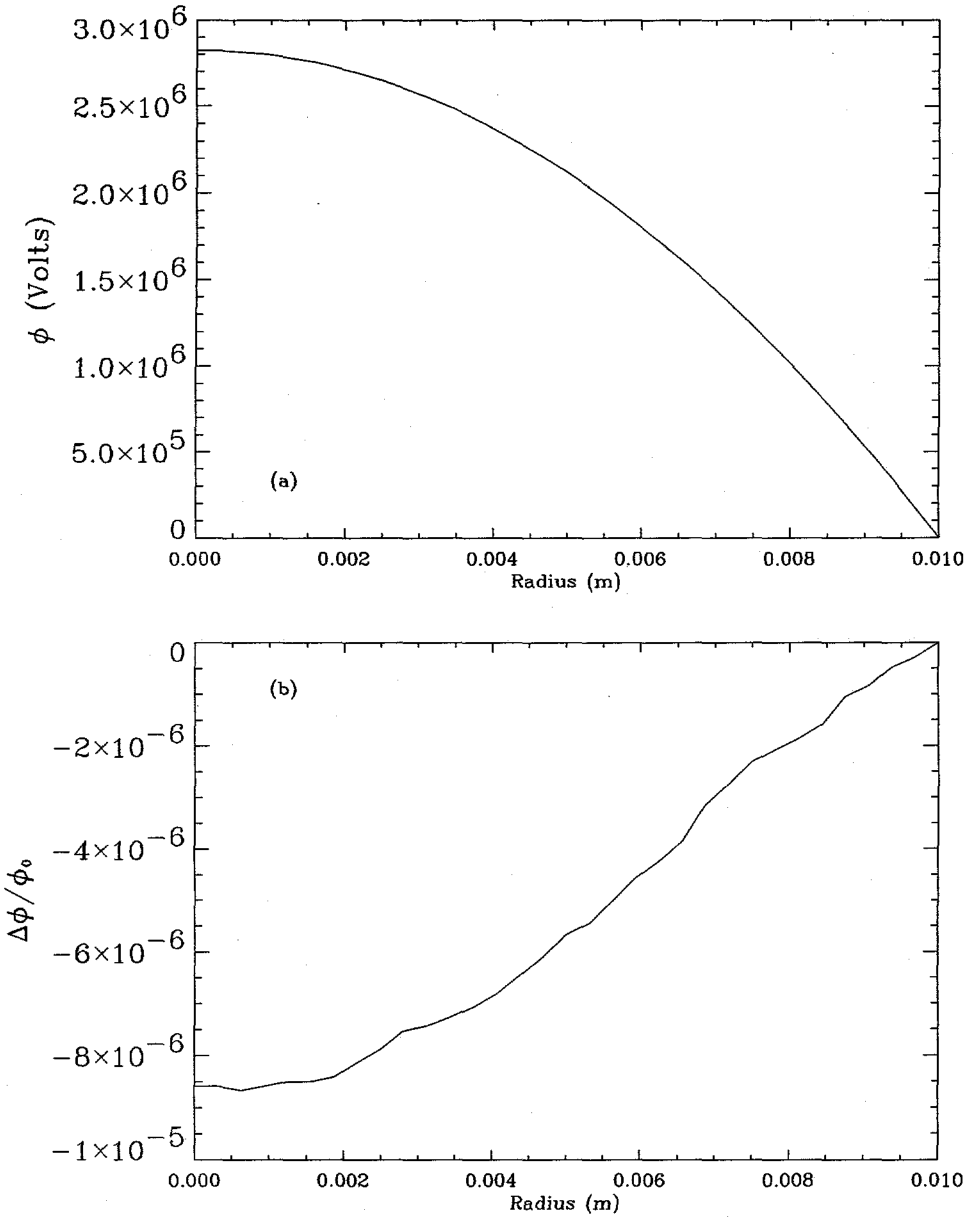

Figure 1: Figure 1(a) shows a plot of $\phi(r)$ obtained from Eq. (23). Figure 1(b) shows the difference between the potential calculated using the Poisson solver and by using Eq. (23) normalized to the theoretical potential at $r = 0$.

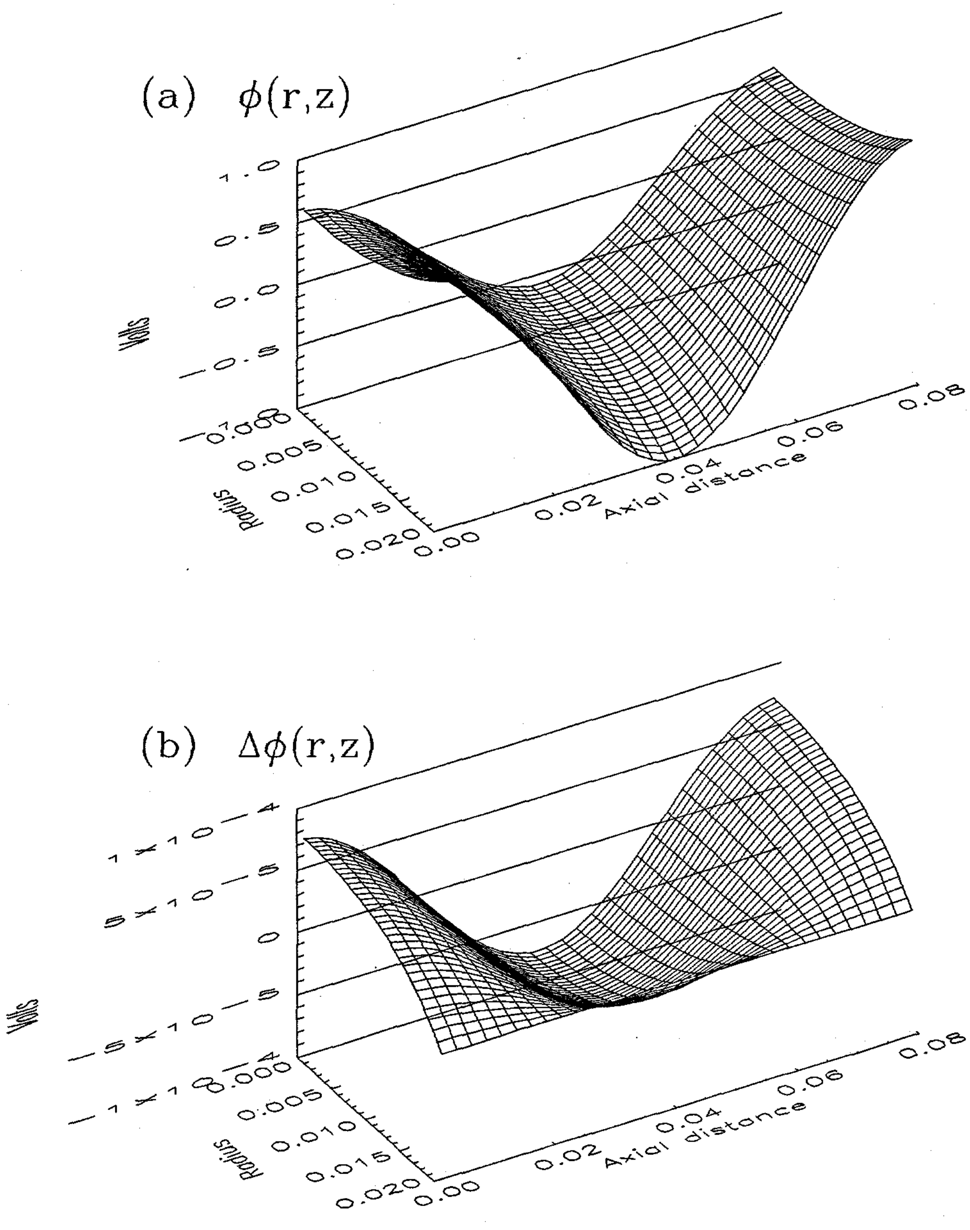

Figure 2: Figure 2(a) shows a plot of $\phi(r,z)$ in Eq. (24) with $V_0 = 1V$, $R_{wall} = 0.02\,m$ and $L = 0.08\,m$. Figure 2(b) shows the difference between the potential calculated using the Poisson solver and by using Eq. (24).