Inversion of the Helmholtz (or Laplace-Poisson) Operator for Slab Geometry

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Presented in this article is a convenient method for determining static or propagating fields due to a slab-confined source distribution. The "propagating" version was developed with a view to studying thin plasma layers (such as the geomagnetic tail or current sheets for fusion machines). The "static" version has been in use for several years to study anomalous plasma diffusion, or electrostatic sheath problems. However, there are numerous other applications: fluid-dynamics, diffraction, radiation from phased arrays, to name but a few.

The significant feature of the geometry is that the source is infinite in two dimensions (y and z) and in time (the case of radiation at steady frequency is of interest), so that Fourier transforming is the obvious treatment for these three variables, but in the remaining single space dimension x, only a finite range has to be covered, with free-space boundary conditions at each end (see Fig. 1).

Fourier-transforming in x is not appropriate: a progressive integration of the ordinary differential equation (Ψ = potential, σ = source):

$$(d^2\Psi/dx^2) + \omega^2\Psi = \sigma \tag{1}$$

is faster and allows the imposition of free-space boundary conditions with great ease. For the two-dimensional Poisson operator, our method therefore resembles that described as "FACR" in Hockney's survey [1].

For the one-dimensional wave equation, ω is the frequency, if one uses units such that the phase velocity is unity. For three-dimensional waves with $e^{i(k_yy+k_zz-\omega t)}$ as the factor designating the Fourier component under consideration, we define ω^2 as a replacement of $\omega^2 - k_y^2 - k_z^2$. In this case one can have negative ω^2 (which one may prefer to write as $-k^2$ for better familiarity), and the case of Laplace's operator, or the Poisson equation, is then included.

The x-interval is broken into finite steps smaller than $1/\pi$ of the smallest wave-

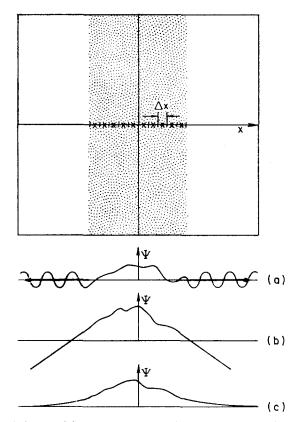


FIG. 1. Potential due to slab-confined source: (a) outward propagating, $\omega^2 > 0$; (b) symmetrically sloping, $\omega^2 = 0$; (c) outward decaying, $\omega^2 < 0$.

length to be handled (i.e., smaller than $2/\omega$). The numbering should be odd, i.e., Ψ and σ are recorded at x-values:

$$\cdots - \frac{5}{2}\Delta x, - \frac{3}{2}\Delta x, - \frac{1}{2}\Delta x, \frac{1}{2}\Delta x, \frac{3}{2}\Delta x, \frac{5}{2}\Delta x \cdots$$

with x = 0 midway between the outer bounds of the source distribution. We use Δx as unit of length. The finite difference equation corresponding to (1),

$$\Psi_{n+1} + \Psi_{n-1} - (2 - \omega^2)\Psi_n = \sigma_n , \qquad (2)$$

could, in principle, be solved by Gauss elimination, but a marching method allows

us better to apply the boundary conditions at $\pm \infty$. With a view to convenient indexing in Fortran, let us define two (complex) arrays

$$\begin{aligned} \Psi_{1^{+}} &= \Psi(\frac{1}{2} \Delta x), \qquad \Psi_{1^{-}} &= \Psi(-\frac{1}{2} \Delta x) \\ \Psi_{2^{+}} &= \Psi(\frac{3}{2} \Delta x), \qquad \Psi_{2^{-}} &= \Psi(-\frac{3}{2} \Delta x) \\ \vdots \\ \text{etc.}, \end{aligned}$$

and similarly for σ . Then (2) is the correct recurrence relation for both Ψ^+ and Ψ^- , provided one interprets: $\Psi_0^+ = \Psi_1^-, \Psi_0^- = \Psi_1^+$.

We let n = N be the largest index for which σ_n^+ or σ_n^- is nonzero, i.e., the source distribution is confined to $|x| < N \Delta x$. To solve (2), we factorize:

$$(\Psi_{n+1}-e^{i\kappa}\Psi_n)-e^{-i\kappa}(\Psi_n-e^{i\kappa}\Psi_{n-1})=\sigma_n$$

where $e^{i\kappa} - e^{-i\kappa} = 2 - \omega^2$ on $\sin(\kappa/2) = \omega/2$. Note that κ is either real (our restriction on Δx ensures that ω is less than 2) or pure imaginary (ω^2 negative). Defining

$$\Phi_n \equiv \Psi_n - e^{i\kappa}\Psi_{n-1},$$

one first solves for Φ_n by an inward march of

$$\Phi_n = (\Phi_{n+1} - \sigma_n) e^{i\kappa} \quad \text{from } n = N \text{ down to } n = 1, \tag{3}$$

and then for Ψ_n by an outward march of

$$\Psi_n = \Phi_n + e^{i\kappa}\Psi_{n-1}$$
 from $n = 1$ to $n = N$. (4)

The question is how to begin these marches: what do we use for Φ_{N+1} in (3) and what do we use for Ψ_0 in (4)? Suppose we took the recurrence relation out into the source-free region n > N, where $\sigma_n = 0$. Then (3) would have the solution $\Phi_n = Ae^{-i\kappa n}$ where A = const and, inserting this into (4), one gets

$$\Psi_n = A e^{-i\kappa n} / (1 - e^{2i\kappa}) + B e^{i\kappa n}, \tag{5}$$

where B is some other constant. Here the first term, coupled with the time factor $e^{-i\omega t}$, represents an incoming wave not admissable for causality reasons if Ψ is to represent the potential due to the source σ alone (Fig. 1a). Hence A = 0 and $\Phi_n = 0$ in the source-free exterior, so that

$$\Phi_{N+1} = 0 \tag{6}$$

for the start of the inward march.

In the case where ω^2 is negative, as it certainly will be for the 2- or 3-dimensional Laplace/Poisson problem, we choose a positive imaginary ω so that we get a positive imaginary κ . This has the effect of stabilizing both marches (3) and (4), in that each next value is obtained by multiplying with a number less than unity: errors are knocked down. It also results (Fig. 1c) in the exclusion of the first term in (5) which represents an outward increasing potential. The choice A = 0 and (6) for Φ_{N+1} is the correct choice, albeit for different reasons. In this case, incidentally, one would not represent the multiplier in (3) and (4) as an exponential but as that solution of the quadratic $(e^{i\kappa}) + 1/(e^{i\kappa}) = 2 - \omega^2$ which is less than unity.

What we have found so far applies both to the potentials Ψ^+ with their sources σ^+ on the right and to the potentials Ψ^- with their sources σ^- on the left. The corresponding Φ^+ and Φ^- can both be marched inwards simultaneously starting from $\Phi^{\pm}_{N+1} = 0$.

To start the outward march, we determine Ψ_0^+ and Ψ_0^- from the consistency of the two conditions

$$\begin{aligned} \Psi_{0}^{+} &= \Psi_{1}^{-} = \Phi_{1}^{-} + e^{i\kappa}\Psi_{0}^{-} \\ \Psi_{0}^{-} &= \Psi_{1}^{+} = \Phi_{1}^{+} + e^{i\kappa}\Psi_{0}^{+} \end{aligned} \tag{7}$$

i.e., from joining the solutions in the middle of the slab. From (7) we find

$$\Psi_1^{+} = (\Phi_1^{+} + e^{i\kappa}\Phi_1^{-})/(1 - e^{2i\kappa})$$
(8)

$$\Psi_1^- = (\Phi_1^- + e^{i\kappa}\Phi_1^+)/(1 - e^{2i\kappa}) \tag{9}$$

which allows us to begin the outward marches of Ψ_n^+ and Ψ_n^- now with n = 2. The case of the vanishing denominator is taken up below.

The program, then, consists of the reverse loop (3), initialized by (6), with + and - superscripted variables processed simultaneously, then the pair of statements (8, 9) and finally the forward loop (4), again with + and - variables processed simultaneously beginning with n = 2. In the loops, Φ_n^{\pm} can overwrite σ_n^{\pm} and Ψ_n^{\pm} can overwrite Φ_n^{\pm} .

Here, as in the FFT's for transforming the variables y, z, and t, one can avail oneself of a trick to speed up the complex multiplications in those machines which take longer to multiply than to add: Along with $S = \sin \kappa$ one stores $T = \tan(\kappa/2)$ rather than $C = \cos \kappa$. The complex multiplication U + iV = (C + iS) * (X + iY) (four real multiplications and two real additions) then becomes:

$$U' = X - T * Y$$
$$V = Y + S * U'$$
$$U = U' - T * V$$

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(three real multiplications and three real additions). The prime may be omitted in Fortran.¹ On an IBM 360/65 this gives a 15% saving per complex multiplication.

The case of the vanishing denominator in (8, 9), $\kappa = 0$, has still to be dealt with. The one-dimensional Poisson problem falls into this category.

Outside the source distribution Ψ must be linear in this case (Fig. 1b). Φ represents the potential gradient and one cannot discriminate against a nonzero gradient for $n \ge N + 1$. Let us, nevertheless, build up Φ^+ and Φ^- by simultaneous inward marches starting with $\Phi_{N+1}^{\pm} = 0$. These inward marches may then finish with possibly contradictory values Φ_1^+ and Φ_1^- in that (7) now states

$$\Phi_1^{+} = \Psi_0^{+} - \Psi_0^{-} \tag{10}$$

$$\Phi_1^- = \Psi_0^- - \Psi_0^+. \tag{11}$$

We note from (3) with $e^{i\kappa} = 1$ that $-\Phi_1^+$ and $-\Phi_1^-$ represent the totals of the source strengths ("charge" in the electrostatic interpretation) on the right and left respectively. Thus (10) and (11) are compatible only provided the total source strength *overall* is zero. Otherwise, we must correct all Φ 's by subtracting a uniform gradient γ given by

$$\gamma = \frac{1}{2}(\Phi_1^+ + \Phi_1^-),$$

from all Φ -values created in the inward march. One does this by subtracting γ at each step of the outward march.

The start of the latter is not uniquely determined, since one can choose an arbitrary zero of potential, but the choice

$$\Psi_{0}^{+} = \frac{1}{2}(\Phi_{1}^{+} - \Phi_{1}^{-}) = -\Psi_{0}^{-},$$

compatible with (10) and (11), is as good as any: it places the potential zero in the middle.

The slopes of potential outside the source distribution are now the same in magnitude and opposite in direction on the two sides of the slab: the potential is that due to the slab alone in free space, symmetric at large distances (Fig. 1b).

Apart from its intrinsic convenience, the marching method described here greatly facilitates the introduction of internal boundaries at fixed potentials (e.g., an array of finite-diameter grid wires in the two-dimensional electrostatic problem).

In this case one uses the "capacitance matrix" method developed at Stanford and described by Hockney [1]. One solves without paying any attention to the

¹ The symbol "*" is here used to indicate multiplication, in order to emphasize that we are concerned with a computing algorithm. Note incidentally that the Fortran statement Z = E * Z where Z = X + iY and E = C + iS can be executed as X = X - T * Y, Y = Y + S * X, X = X - T * Y.

internal boundaries in the first place and one ignores any possible surface charges that would develop on the internal conductors. This is step "A." Then, in step "B," one determines the amounts by which the resulting surface potentials fail to meet the imposed conditions. In step "C" one multiplies the potential deficiencies into the capacitance matrix to determine the required surface charges and in step "D" one solves the potential problem again, this time including the surface charges.

The point is that one can place the middle of the slab, x = 0, at or near the median plane of all internal boundaries, so that the latter cover only a minimal range from the center rightward and leftward (see Fig. 2). In step "A" one now only

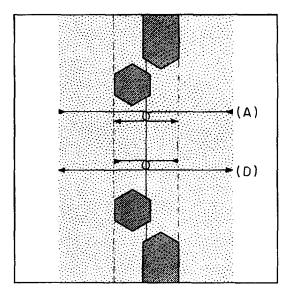


FIG. 2. Marches in the presence of internal boundaries: (A) before knowledge of surface charges, (D) after evaluation of surface charges.

marches inwards and part of the way outwards, namely to the outermost point of the internal boundaries. Only for this last short range need one Fourier-invert the Ψ -values in order to determine the potential deficiencies in step "B." For step "D" one can then pick up the original inward march at the edge of the internal boundaries, make a brief double march in the innermost region, then create the Ψ 's all the way to the end of source distribution (see Fig. 2).

The algorithms and special tricks described in this note have all been used and tested. Further applications, particularly to cylindrical (rather than slab) geometry, using conformal mapping, and to radiation, are in progress.

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References

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