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Note

Analytic Inversion of the Five-Point Poisson Operator*

There are situations when the potential due to a single line charge in an unbounded domain is of interest, and when this potential is to be the solution of a finite-difference Poisson operator and not that of the ∇^2 operator.

For instance, one may wish to study self-forces resulting from specific charge sharing [1] and interpolation schemes [4] applied to a potential due to, say, a five-point numerical Poisson solver.

Also, if one has to simulate infinite space conditions on a finite boundary [2], one may wish to precalculate potentials on that boundary from the charge distribution by direct application of a kernel, prior to filling in the interior potential values with the aid of a five-point finite-difference finite-domain Poisson solver.

Furthermore, it is of interest to know exactly what potentials ought to be added to a distribution reached in the course of relaxation, in order to compensate a single residue at a large distance from any boundary.

Lastly, one may like to have the standard ideal potential pattern (in the close vicinity of a single line charge) available for checking a program which is intended to solve the 5-point Poisson formula. (See Ref. [3] for a survey of Poisson solvers.)

This pattern is shown in Tables I and II. The line charge is -1 (Gaussian units) and is in the top left corner where the potential zero has been placed. At large distances the potential approaches $2(\ln r + \text{constant})$ as for the ∇^2 operator. The "constant" is $(3/2)\ln 2 +$ Euler's constant when r is measured in cell mesh units.

The important thing to realize is that Table I was obtained analytically and not by a numerical Poisson solver. Table II is Table I with substitutions for π. Since there are no rigorous numerical 5-point Poisson solvers for an infinite domain, it was necessary to solve the finite difference formula analytically.

The values π in the cells immediately adjacent to the charge are trivial: assuming the finite difference formula

$$4\Phi_{\text{center}} - \Phi_{\text{north}} - \Phi_{\text{east}} - \Phi_{\text{south}} - \Phi_{\text{west}} = 4\pi \cdot \text{charge},$$

taking the charge $= -1$, $\Phi_{\text{center}} = 0$ and $\Phi_{\text{north}} = \Phi_{\text{east}} = \Phi_{\text{south}} = \Phi_{\text{west}}$ by symmetry, it follows that the common value of these four potentials is π.

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TABLE I

Potentials Created by a Negative Gaussian Unit of Charge in the Top Left Corner

0	π	$4\pi - 8$	$17\pi - 48$	$80\pi - 245\frac{1}{3}$
π	4	$-\pi + 8$	$-8\pi + 30\frac{2}{3}$	$-49\pi + 160$
$4\pi - 8$	$-\pi + 8$	$5\frac{1}{3}$	$\pi + 2\frac{2}{3}$	$12\pi - 31\frac{7}{15}$
$17\pi - 48$	$-8\pi + 30\frac{2}{3}$	$\pi + 2\frac{2}{3}$	$6\frac{2}{15}$	$-\pi + 9\frac{3}{5}$
$80\pi - 245\frac{1}{3}$	$-49 + 160$	$12\pi - 31\frac{7}{15}$	$-\pi + 9\frac{3}{5}$	$6\frac{74}{105}$

TABLE II

Decimal Equivalent of Table I. In Brackets: Deviations of Values from Those Obtained by the Logarithmic Formula

0	3.1416	4.5664	5.4071	5.9941
(∞)	(-0.0923)	(-0.0538)	(-0.0240)	(-0.0124)
3.1416	4.0000	4.8584	5.5339	6.0620
	($+0.0730$)	($+0.0151$)	(-0.0026)	(-0.0051)
4.5664	4.8584	5.3333	5.8082	6.2324
		($+0.0200$)	($+0.0093$)	($+0.0028$)
5.4071	5.5399	5.8082	6.1333	6.4584
			($+0.0090$)	($+0.0056$)
5.9941	6.0620	6.2324	6.4584	6.7048
				($+0.0051$)

What is not at all obvious is the sequence of rational numbers along the diagonal, namely,

$$0,\ 4,\ 4 + 4/3,\ 4 + 4/3 + 4/5,\quad \text{etc.}$$

We note, first, that these values give the correct field at points midway between cell centers, i.e., at cell corners, if simple diagonal differencing is used there: at distance $r = (2n - 1)\sqrt{2}/2$ we get a field $4/(2n - 1)\sqrt{2} = 2/r$. This singularly good performance of the 5-point scheme is somewhat freakish—it is restricted to just these points along the diagonal.

Having obtained the adjacent values π and the values along the diagonal, one can build up the remainder of the table by applying the five-point operator at a judiciously chosen succession of mesh points: for instance, the value $4\pi - 8$ in in the top line or left column follows from applying the five-point operator at the "π" points and using the pattern symmetry. The multipliers of π at every grid point are clearly integers. The denominators of the rational contributions propagate diagonally as shown in Table I.

To account for the diagonal sequence, we employ what is probably the most successful method for building a fast Poisson solver [3], namely, Fourier analysis in one dimension (the North–South direction) together with solving a three-term recurrence relation in the other dimension (East–West). In the first place we impose a periodicity of N mesh points in the North–South direction, but since our results are analytical, we can let N tend to infinity in due course. We define Fourier transforms

$$\tilde{\Phi}_k^{(m)} = \sum_{k=1-N/2}^{N/2} \Phi_n^{(m)} e^{-2\pi i k n/N},$$

where n is the index running along a column (N–S) while m runs across (E–W). The negative unit charge at $n = 0$, $m = 0$, has all transforms -1 for $m = 0$, zero for $m \neq 0$.

For the k-th harmonic we have $\Phi_{\text{north}} + \Phi_{\text{south}} = 2\Phi_{\text{center}} \cos(2\pi k/N)$ and the recurrence formula becomes:

$$\tilde{\Phi}_k^{\text{east}} + \tilde{\Phi}_k^{\text{west}} + \tilde{\Phi}_k^{\text{center}}[2 \cos(2\pi k/N) - 4] = 0$$

except when "center" refers to the column $m = 0$. In that case the right side is 4π. The solution is, for $k \neq 0$,

$$\tilde{\Phi}_k^{(m)} = \tilde{\Phi}_k^{(0)}/K^{|m|},$$

where K is obtained from k as that root of the quadratic

$$K + 1/K = 4 - 2 \cos 2\pi k/N,$$

which is greater than unity. By making $\tilde{\Phi}_k^{(m)}$ decay with $|m|$, i.e., in both the positive and the negative direction, we ensure free-space boundary conditions in the East–West dimension. Solution of the recurrence relation which increase outward, or any admixture of such a solution, are not admissible.

Taking "center" at $m = 0$ we now get a condition for $\tilde{\Phi}_k^0$, namely

$$[(2/K) + 2 \cos(2\pi k/N) - 4]\, \tilde{\Phi}_k^0 = 4\pi,$$

or, with substitution from the equation defining K,

$$\tilde{\Phi}_k^{(0)} = \frac{-4\pi}{K - 1/K}.$$

Special treatment is needed for the component $k = 0$ (uniformity in the N–S direction). This component, according to the recurrence relation for $m \neq 0$, has to vary linearly with m and, matching across $m = 0$, one gets

$$\tilde{\Phi}_0^{(m)} = 2\pi |m|$$

rising symmetrically towards East and West. This choice implies that the periodic array of negative charges is solely responsible for the field, and that no external field is applied at infinity. It also implies a potential zero mean on $m = 0$.

Now we are ready to back-transform:

$$\tilde{\Phi}_n^{(m)} = \frac{1}{N} \sum_{1-N/2}^{N/2} e^{2\pi i k n/N} \tilde{\Phi}_n^{(m)} = \frac{2\pi \mid m \mid}{N} - \frac{4\pi}{N} \sum_{1-N/2}^{N/2\prime} \frac{e^{2\pi i k n/N}}{K^{\mid m \mid}(K - 1/K)},$$

where the prime in the summation indicates omission of the term $k = 0$.

The potential relative to the origin ($n = 0$, $m \neq 0$) is

$$\Phi_n^{(m)} - \Phi_0^{(0)} = \mid m \mid \delta\theta - 2 \sum{}' \left(\frac{e^{i\theta n}}{K^{\mid m \mid}} - 1 \right) \frac{\delta\theta}{K - 1/K},$$

where we have defined the angle

$$\theta = 2\pi k/N$$

and its increment

$$\delta\theta = 2\pi/N,$$

so that we may now let N tend to infinity, with θ becoming a continuous variable and the summation becoming an integration:

$$\Phi_n^{(m)} - \Phi_0^{(0)} = -2 \int_{-\pi}^{+\pi} \left(\frac{e^{i\theta n}}{K^{\mid m \mid}} - 1 \right) \frac{d\theta}{K - 1/K}.$$

The exclusion of $\theta = 0$ from the summation becomes ignorable in the limit since the integrand remains well behaved and finite as $\theta \to 0$. Since K is an even function of θ, we can halve the range of integration:

$$\Phi_n^{(m)} - \Phi_0^{(0)} = 4\mathrm{Re} \int_0^{\pi} \left(1 - \frac{e^{i\theta n}}{K^{\mid m \mid}} \right) \frac{d\theta}{K - 1/K}.$$

Trigonometric integrals are evaluated by introducing the tangent of the half-angle:

$$t = \tan \theta/2,$$

$$d\theta = \frac{2dt}{1 + t^2},$$

$$0 \leqslant t \leqslant \infty,$$

$$e^{i\theta} = (1 + it)/(1 - it),$$

$$K = [3t^2 + 1 + 2t \sqrt{(2t^2 + 1)}]/(1 + t^2),$$

$$d\theta/(K - 1/K) = dt/[2t \sqrt{(2t^2 + 1)}].$$

A further standard transformation removes the square roots:

$$t = \sqrt{2}\,\tau/(1-\tau^2),$$

$$dt = \sqrt{2}\{(1+\tau^2)/[(1-\tau^2)^2]\}\,d\tau,$$

$$0 \leqslant \tau \leqslant 1.$$

$$\sqrt{(2t^2+1)} = (1+\tau^2)/(1-\tau^2),$$

$$dt/2t\sqrt{(2t^2+1)} = d\tau/2\tau,$$

$$e^{i\theta} = (\tau-\sqrt{i})(\tau+\sqrt{-i})/(\tau+\sqrt{i})(\tau-\sqrt{-i}),$$

$$K = \frac{(\tau^2+\sqrt{2}\,\tau+1)^2}{\tau^4+1} = \frac{\tau^2+\sqrt{2}\,\tau+1}{\tau^2-\sqrt{2}\,\tau+1} = \frac{(\tau+\sqrt{i})(\tau+\sqrt{-i})}{(\tau-\sqrt{i})(\tau-\sqrt{-i})},$$

where $\sqrt{\pm i} \equiv (1 \pm i)/\sqrt{2}$ so that

$$\Phi_n^{(m)} - \Phi_0^{(0)} = 4\mathrm{Re}\int_0^1 \left(1 - \left(\frac{\tau-\sqrt{i}}{\tau+\sqrt{i}}\right)^{n+|m|}\left(\frac{\tau+\sqrt{-i}}{\tau-\sqrt{-i}}\right)^{n-|m|}\right)\frac{d\tau}{2\tau}.$$

(Here we readily verify that $\tau = 0$ is not a singularity of the integrand.)

The evaluation of all potentials has thus been reduced to integrations of rational functions. We are interested in the diagonal terms where $n = |m|$ and, more specifically, the potential differences along the diagonal:

$$\Phi_n^{(n)} - \Phi_{n-1}^{(n-1)} = 4\mathrm{Re}\int_0^1 \left[\left(\frac{\tau-\sqrt{i}}{\tau+\sqrt{i}}\right)^{2n-2} - \left(\frac{\tau-\sqrt{i}}{\tau+\sqrt{i}}\right)^{2n}\right]\frac{d\tau}{2\tau}$$

$$= 4\mathrm{Re}\int_0^1 \frac{2\sqrt{i}(\tau-\sqrt{i})^{2n-2}}{(\tau+\sqrt{i})^{2n}}\,d\tau$$

$$= 4\mathrm{Re}\left[\left(\frac{\tau-\sqrt{i}}{\tau+\sqrt{i}}\right)^{2n-1}\right]_0^1 \Big/ (2n-1),$$

as can be verified by direct differentiation. At the upper limit, the square bracket is pure imaginary, as can be seen from applying Thales' theorem to the triangle $\sqrt{i}$, 1, $-\sqrt{i}$ inscribed into the unit circle. At the lower limit, one gets -1 and, hence,

$$\Phi_n^{(n)} - \Phi_{n-1}^{(n-1)} = 4/(2n-1),$$

as used in the table. The potential at distance $r = n\sqrt{2}$ along the diagonal is

$$\begin{aligned} &4[1 + 1/3 + 1/5 + \cdots + 1/(2n-1)] \\ &\quad = 4(1 + 1/2 + 1/3 + \cdots + 1/2n) - 2(1 + 1/2 + 1/3 + \cdots + 1/n) \\ &\quad = 4(\ln(2n) + \gamma) - 2(\ln n + \gamma) = 2(\ln n + \gamma + \ln 2) \\ &\quad = 2(\ln r + \gamma + (3/2)\ln 2). \end{aligned}$$

The table of potentials to compensate a unit residue in a relaxation algorithm can be obtained from Table I or II by complementing it with the boundary potential. Let us suppose that the boundary is circular about the origin and a little over 100 mesh lengths away, 106, to be precise. Then $\ln r + \gamma + (3/2) \ln 2 = 6.2832 = 2\pi$ at the boundary, so that the table of compensatory potentials consists of 4π minus the potentials in Table II. This is for a unit residue in Gaussian units. Since relaxation is normally carried out in "rational" or "Heaviside" units, not including the factor 4π, one gets Table III for the close vicinity of a unit residue to be compensated.

TABLE III

Potentials to Compensate Unit Residue at Top Left Corner with Boundary 106 Mesh Units Away. Values Beyond Range of Table are Less Than 0.5

1.00	0.75	0.64	0.57	0.52
0.75	0.68	0.61	0.56	0.52
0.64	0.61	0.58	0.54	0.50
0.57	0.56	0.54	0.51	0.49
0.52	0.52	0.50	0.49	0.47

In view of the large area covered by nonnegligible and smoothly varying values in Table III it is suprising that the old scheme of compensating a residue by a few local potential corrections ever worked.

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