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Inversion of Lewis' Poisson Operator

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After performing the inversion of a 5-point Poisson operator [1] and a 9-point Poisson operator [2] analytically, an attempt was made to do the same thing for the "optimal" Poisson operator that goes with parabolic splines. Lewis' variational principle [3] prescribes such an operator uniquely. Preference was given to parabolic splines because in all probability the computationally more costly higher order splines will not be used for potential evaluations on a production basis.

The 5-point operator is constructed from the requirement that it should be exact for potential distributions that are cubic in x and y and hence for linear charge distributions.

The 9-point operator springs from the requirement that fifth order potentials, or cubic charge distributions, should be handled accurately.

Lewis' operator connects an array of spline coefficients for the potential with a charge distribution which is itself a superposition of splines. Both sets of splines are taken of the same order—parabolic by our choice. These splines have the profile

$$\begin{array}{ll} \frac{1}{2}(\frac{3}{2}+x)^2 & -\frac{3}{2} \leqslant x \leqslant -\frac{1}{2} \\ \frac{3}{4}-x^2 & -\frac{1}{2} \leqslant x \leqslant \frac{1}{2} \\ \frac{1}{2}(\frac{3}{2}-x)^2 & \frac{1}{2} \leqslant x \leqslant \frac{3}{2} \end{array} \tag{1}$$

and zero elsewhere.

(Three parabolic segments are joined smoothly to each other and to the horizontal axis at the ends, forming a bell-shaped curve overall.)

Inserting the spline profile (1) into Eq. (50) of Lewis' paper on the variational technique [3], one obtains a *one*-dimensional *five*-point Poisson operator with coefficients 1/6, 1/3, −1, 1/3, 1/6. This was used by Lewis himself in some preliminary tests of his scheme [4] and transformed into Fourier space by Langdon [5], who also draws attention to the factorization of this operator, i.e., it can be represented as $\delta^2(1 + \delta^2/6)$ where δ^2 is the second-order central difference operator.

In two dimensions we have to use Eq. (63) of Lewis' paper [3] and we obtain a 25-point operator with the coefficients

$$\frac{1}{360}\begin{pmatrix} 1 & 14 & 30 & 14 & 1 \\ 14 & 52 & -12 & 52 & 14 \\ 30 & -12 & -396 & -12 & 30 \\ 14 & 52 & -12 & 52 & 14 \\ 1 & 14 & 30 & 14 & 1 \end{pmatrix},$$

more convincingly expressed in central difference notation:

$$(\delta_x^2 + \tfrac{1}{6}\delta_x^4)(1 + \tfrac{1}{4}\delta_y^2 + \tfrac{1}{120}\delta_y^4) + \text{same with } x \text{ and } y \text{ reversed.}$$

Symbolically, we can invert this operator by writing it as a denominator, and we might then compare it with, say, the corresponding symbolic inverse 5-point and 9-point operators of [1, 2], namely,

$$P_5 = 1/(\delta_x^2 + \delta_y^2), \tag{2}$$

$$P_9 = 1/(\delta_x^2 + \delta_y^2 + \delta_x^2\delta_y^2/6) + (1/12). \tag{3}$$

(The denominator in P_9 is readily checked to be the central-difference representation of the coefficients for the 9-point operator given in [7].)

However, there is a difference between the function of the Lewis operator and that of the two others. P_5 and P_9 generate arrays of potentials from arrays of density. Lewis' operator generates an array of spline coefficients for the potential. To get, instead, the potential array itself, we have to apply the three weights, 1/8, 3/4, 1/8 at $x = -1$, 0 and 1 of the profile (1) to all entries of the spline coefficient array. This amounts to operating on the array with $1 + \delta^2/8$, and it must be done in two dimensions, meaning that $(1 + \delta_x^2/8)(1 + \delta_y^2/8)$ should be applied.

Furthermore, the spirit of Lewis' scheme [3] is to spread any single charge into a cloud with the profile (1) in both dimensions in order to generate an array of gridpoint density values. An array of charges located exactly at the gridpoints will therefore be spread into the density array given, again, by application of the operator $(1 + \delta_x^2/8)(1 + \delta_y^2/8)$.

Combining the two considerations of the two preceding paragraphs, we see that for a comparison of P_5 and P_9 with the Lewis operator, we ought to employ a numerator $(1 + \delta_x^2/8)^2(1 + \delta_y^2/8)^2$ when symbolically inverting the latter:

$$P_L = \frac{(1 + \delta_x^2/8)^2\,(1 + \delta_y^2/8)^2}{(\delta_x^2 + \delta_x^4/6)(1 + \delta_y^2/4 + \delta_y^4/120) + \text{same with } x, y \text{ reversed}}. \tag{4}$$

The logic of having to apply the operator $(1 + \delta_x^2/8)(1 + \delta_y^2/8)$ twice directly in order to get from an array of discrete charges to an array of actual potentials may seem strange. One is tempted to apply this operator inversely on one of these occasions and hence to cancel the two operations against each other. However, one can convince oneself that the original prescription is correct by following Lewis' rules [3] for finding the potential anywhere between gridpoints due to a charge located away from any gridpoints, and then letting both the point of observation and the charge approach a gridpoint.

Our aim is to evaluate the inverse Lewis operator which is formally written down in 4. By this we mean tabulation of the corresponding kernel or "Greens function", such as given for the 5-point and 9-point operators in Refs. [1, 2]. There seems to be little hope of success with the method used for the inversion of the 5-point and 9-point operators, i.e., Fourier transforming in one dimension and solving a recurrence relation in the other.

Instead, we try Fourier transforms in both dimensions. Starting with a large periodicity square consisting of N-by-N gridpoints, and with the harmonic which varies like $\exp(2\pi i(Kx + Ly)/N)$, one obtains the numbers

$$\delta_x^2 = -(2 \sin \pi K/N)^2, \qquad \delta_y^2 = -(2 \sin \pi L/N)^2$$

for the central difference operators, and each of our three inverse Poisson operators, P_5, P_9 and P_L, becomes a K- and L-dependent number.

For an isolated negative gaussian unit charge at the origin the double Fourier transform of $\nabla^2\Phi$ is independent of K and L, namely, $4\pi/N^2$. Multiplying by one of the operators P and back-transforming, we get the following potential *relative to the origin*:

$$\Phi(x, y) = \frac{1}{\pi} \sum_{1-N/2}^{N/2} \sum_{1-N/2}^{N/2} P(K, L)(e^{2\pi iKx/N}e^{2\pi iLy/N} - 1)\left(\frac{2\pi}{N}\right)^2.$$

Since P is even in K and L, the (odd) imaginary parts of the exponentials can be ignored, leaving only the cosines.

All three P's become large like $-(N/2\pi)^2/(K^2 + L^2)$ for small K and L. It is convenient to avoid these large numbers in the numerical evaluation of the double sum, even though they are compensated by the factor containing the exponentials or cosines. Since we have already calculated Φ for the 9-point operator analytically [2], we may subtract the 9-point results and concern ourselves only with the difference

$$\Phi_L - \Phi_9 = \frac{1}{\pi} \sum_{1-N/2}^{N/2} \sum_{1-N/2}^{N/2} (P_L - P_9)\left(\cos \frac{2\pi Kx}{N} \cos \frac{2\pi Ly}{N} - 1\right)\left(\frac{2\pi}{N}\right)^2.$$

This difference was evaluated for integer x and y ranging each from 0 to 3, using $N = 256$. The results are shown in Table I below. Using $N = 128$ gave the same results to eight digits accuracy, so that the periodicity cell had been taken

TABLE I

Difference between Lewis potentials and 9-point potentials relative to infinity ($\Phi_L - \Phi_9 - 0.19493$)

−0.19493	0.07620	−0.03396	0.01016
	−0.01314	0.00897	−0.00432
		−0.00113	0.00143
			−0.00025

large enough. In fact, the double sum is an adequate approximation to the ideal double integral obtained by defining $k = 2\pi K/N$, $l = 2\pi L/N$, $\delta k = \delta l = 2\pi/N$ and letting N tend to infinity:

$$\Phi_L - \Phi_9 = \frac{4}{\pi} \int_0^\pi \int_0^\pi (P_L - P_9)(\cos kx \cos ly - 1)\, dk\, dl.$$

Even though $P_L - P_9$ remains moderate as K and L tend to zero, a special algorithm had to be written for evaluating $P_L - P_9$ when both K and L are small, so as to avoid subtraction of nearly equal large numbers. Now the remarkable thing is that an expansion in ascending powers of K and L showed that $P_L - P_9$ is not only finite as $K, L \to 0$, but it is small and of second order in K and L. (Without the numerator $(1 + \delta_x^2/8)^2(1 + \delta_y^2/8)^2$ which we introduced after rather subtle reasoning, this would not have been so.)

A contour map of $P_9 - P_L$ is shown in Fig. 1 over one quadrant of the wave-number plane (K from 0 to 128 across, L from 0 to 128 down). In this display the location (K, L) contains the last hexadecimal place of the integer part of $256(P_9 - P_L)$, provided it is odd. An unreduced version of the diagram permits one to read the characters; they are 1, 3, 5, 7, 9, *B*, *D*, *F*, 1 in the successive bands starting from the top left. The figure shows that nothing much happens until one gets to the harmonics which vary fast enough to reverse sign between adjacent cells. At long and moderate wavelengths the Lewis and 9-point operators give almost indistinguishable results, both coming very close to the ideal logarithmic potential, since both P_9 and P_L differ from the ideal inverse Laplacian, i.e., from $-1/(k^2 + l^2)$, by terms which go to zero quadratically in k and l.

Since $P_L - P_9$ is so smooth, one can deal with the limit $x \to \infty$, $y \to \infty$ by simply omitting the cosines in the double sum above; they average out to zero in this limit. It was found that $\Phi_L - \Phi_9 \to 0.19493$ in this limit. We know [2] that Φ_9, when adjusted to zero at the origin, tends to $ln(x^2 + y^2) + 2\gamma + ln 12 - \pi/3$. Thus Φ_L tends to a limit 0.19493 higher than this expression. In Table I we have deducted 0.19493 throughout, so that the table compares the two potentials relative to infinity, not relative to the origin.

The difference $P_5 - P_9$ is *not* small at the origin of wavenumber space. There

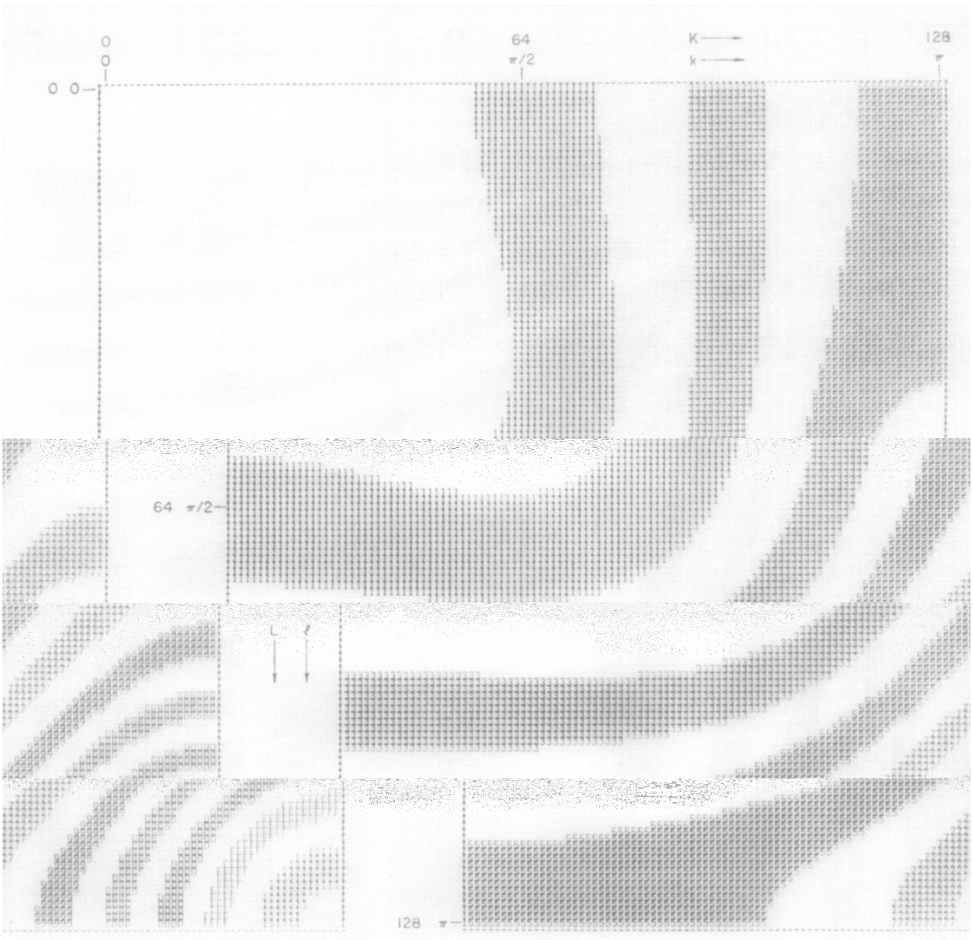

FIG. 1. Fourier transform of difference between 9-point and Lewis inverse operators, P_9–P_L, scaled up by 256. Fourth quadrant of k, l-plane (origin at top left). k and l from 0 to π.

is the k, l-independent term $-1/12$ as well as a term whose behavior is shown in Fig. 2. (Scales as for Fig. 1, the labels of the bands are 1, 3, 5,... F, left to right along the bottom edge.) The origin is singular, and the limiting value of $P_5 - P_9 + \frac{1}{12}$ for $k, l \to 0$, though finite, depends on the direction of approach.

This causes no problems in the evaluations of $\Phi_5 - \Phi_9$ at the low integral x and y values (through 3) for which these evaluations were carried out as "controls". They gave perfect agreement with what can be deduced from the tables of Φ_5 and Φ_9 in Refs. [1, 2].

We note that going along a radius in k, l-space there are no violent variations

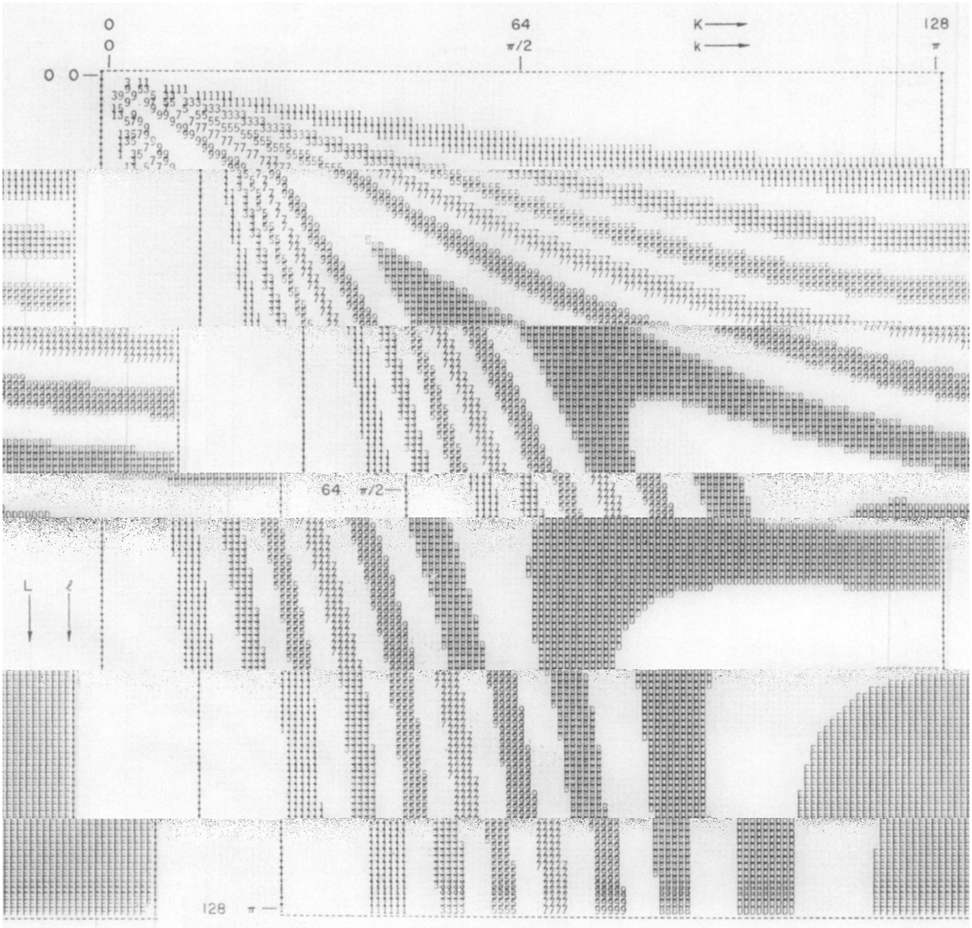

FIG. 2. Fourier transform of difference between 5-point and 9-point inverse operators $P_5 - P_9 + 1/12$, scaled up by 256. Fourth quadrant of k, l-plane, k and l from 0 to π.

in $P_5 - P_9 + 1/12$. Hence one can still get values for $x, y \rightarrow \infty$ by simply omitting the more and more rapidly varying cosine terms in the integral. The remaining integration of $P_5 - P_9 + 1/12$ was carried out numerically (which necessitated a Richardson extrapolation because of the weird behavior of the integrand at the origin). However, it can also be done analytically. Two plausible transformations give the result: First to variables $\xi = \cot k/2$, $\eta = \cot l/2$, and then to polar coordinates in the ξ, η plane. The result is $\Phi_9 - (\pi/3) - \Phi_5 \rightarrow \ln(3/2)$, confirming the ln 12 in the constant of the logarithmic approximation to Φ_9 which had previously been found empirically.

TABLE II

9-point (top line), Lewis (middle line) and 5-point (bottom line) potentials expressed in terms of the logarithmic potential

−2.59214	−0.01174	ln4 −0.00484	ln9 −0.00107
−2.78707	+0.06446	ln4 −0.03880	ln9 +0.00909
−3.23387	−0.09228	ln4 −0.05380	ln9 −0.02402
	ln2 +0.00668	ln5 +0.00139	ln10 −0.00004
	ln2 −0.00646	ln5 +0.01036	ln10 −0.00436
	ln2 +0.07298	ln5 +0.01510	ln10 −0.00253
		ln8 +0.00075	ln13 +0.00027
		ln8 −0.00038	ln13 +0.00170
		ln8 +0.02002	ln13 +0.00944
			ln18 +0.00018
			ln18 −0.00007
			ln18 +0.00909

In Table II we summarize the results for all three operators, using $\ln(x^2 + y^2)$ as reference everywhere except, of course, at the origin. Comparison with the logarithm may be used as a criterion of merit only if one aims at reproducing the potential of a highly concentrated source at the origin. In that case the order of merit seems to be: 5-point—Lewis—9-point; however, along the diagonal the Lewis operator beats the 9-point operator by a small margin. The greatest difference is in the depression at the origin where the 9-point operator, by virtue of being *furthest away* from the logarithmic value $-\infty$, promises least grid noise in particle motion. As explained in [6], the value at the origin can be interpreted as the central potential created by a circular uniform column of charge. In the case of Lewis' operator this column would have to be given a radius of 0.4092 mesh units (as against 0.4511 for the nine-point, 0.3273 for the five-point scheme).

However, the motive for using quadratic splines and optimizing the Poisson operator accordingly is to provide a smooth rather than a spiky density input. It would therefore be more logical to perform tests on smooth density profiles, such as the splines themselves (Eq. (1)), rather than localized sources. These spline profiles should be moved around between grid points. Likewise, the resulting potentials should not be observed at discrete gridpoints: they should be averaged, again with a spline-like profile, over a neighborhood, to see how a smooth distribution of matter responds.

Such tests with smoothed input and output have not yet been made,[1] but per-

[1] The above-mentioned behavior of P_9 and P_L for $k, l \to 0$ indicates that P_9 and P_L will be superior to P_5 at moderate to long wavelengths.

formance on strongly localized sources has been further tested by running the subgrid resolution program of [6] with Lewis' operator in place of the nine-point operator.

In practice, this was achieved by adjusting the potentials read into the subgrid resolution program. The adjustments were those shown in Table I, with extrapolation to the next column (which itself is almost irrelevant in the program). *In effect*, this amounted to (a) finding the weights of the density basis-functions of the form (1) due to an isolated rod anywhere within a cell, (b) inverting the 5-by-5 stencil[2] shown above so as to obtain the array of weights for the potential basis functions, (c) evaluating the quadratic expressions due to superposition of these weighted basis functions, everywhere over a region of 4-by-4 cells.

The final diagrams resemble closely those shown in Ref. [6]. There are one or two more contours owing to the greater well depth (−2.79 in place of −2.59; see Table II) and this makes the distortion for off-grid-point sources more noticeable. The "wobble" in local contours is still of the order of 1/8 mesh unit. Performance on a strongly localized source is decidedly better with the Lewis operator than with the 5-point operator. The latter had been tested in conjunction with quadratic spline fitting in the earliest resolution tests.

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[2] The operator $(1 + \delta_x^2/8)^2(1 + \delta_y^2/8)^2$, included in the calculation of Table I, is removed again by the subgrid resolution program.