DISCUSSION

On: "Numerical integration of related Hankel transforms by quadrature and continued fraction expansion" by A. D. Chave (GEOPHYSICS, 48, p. 1671–1686, December, 1983).

Chave presents an excellent algorithm and computer subprogram that evaluate Hankel transforms by quadrature and continued fraction summation. This subprogram would be a valuable addition to any mathematical computer library. Chave refers to digital filter (convolution) methods as "the standard numerical approach to the computation of Hankel transforms," and makes numerous references to my published work (Anderson, 1979, 1982). However, some readers may misinterpret some of his statements regarding convolution methods, which I hope to clarify by this discussion.

On p. 1671, Chave states (referring to Anderson, 1979) that "Reasonable (5-figure) accuracy is typically achieved for monotonic, rapidly decreasing kernel functions at moderate values of ρ." This statement implies a stronger condition imposed on the kernels than defined in Anderson (1979, p. 1289), where only continuous, bounded kernels are required. Rapid convergence of the convolution sum is achieved if the kernel function is also decreasing (Anderson, 1982), but the rate of decrease is usually immaterial, inasmuch as extremely rapid decaying digital filter responses are used. The 5-figure accuracy is typical of single-precision (32 or 36-bit floating-point) implementations as exemplified in subprograms ZHANKS (Anderson, 1979) and HANKEL (Anderson, 1982), where the best relative errors are approximately 10^{-6}.

Chave's brief reference on p. 1671 to "adaptive and lagged convolution" in Anderson (1982) failed to mention that a double-precision (64-bit floating-point) *related and lagged convolution* subprogram (DHANKL) is available, where best relative errors are approximately 10^{-12}. He further states on p. 1671: "For some types of problems the digital filter method is less useful; examples occur at very small values of the range ρ, ..., and when high numerical precision is required." With either HANKEL or DHANKEL, very small values of $\rho \geq 0$ can be accommodated by lagged convolution as discussed by Anderson (1982, p. 366: "Proceeding to the limit").

In some applications the need for double-precision and very small arguments may be avoided by using suitable transformations of the Hankel integral. For example, the electromagnetic (EM) induction problem discussed by Anderson (1979, p. 1292–1293) used a normalized induction number ($B = \rho/\delta$, where δ is the skin depth of the medium) instead of the usual distance ρ parameter in the Bessel argument of the Hankel transform. This approach usually avoids small transform B arguments, where B is typically in the range [.01, 10] for the quasi-static assumption. Algebraically divergent Hankel transforms of the type discussed by Anderson (1979, p. 1293) and Frischknecht (1967, p. 6–7) can be replaced with rapidly convergent ones by subtracting a known homogeneous half-space term under the integral and adding an equivalent analytic expression outside the integral. For many practical EM problems, combining these two substitutions will result in Hankel transforms that converge rapidly for a moderate induction number range; they are therefore computationally tractable using the single-precision convolution subprograms ZHANKS, HANKEL, or similar routines.

The oscillatory bounded kernels mentioned on p. 1674 can be transformed successfully with moderate to large arguments in ZHANKS, HANKEL, or DHANKL, if the highest frequency content of the kernel function does not approach or exceed the digital filter's sampling or Nyquist frequency (see Anderson, 1982, p. 346, p. 362 regarding oscillating functions). Highly oscillatory kernels are rare in practice, but when they do occur, the quadrature algorithm Chave proposed would generally be more useful and accurate than convolution methods.

On p. 1674, the statement, "Only the first pair of integrals (6)–(7) can be handled by the digital filter method" is misleading in view of the above discussion. Integrals (8)–(9) and (12)–(13) can also be numerically transformed using convolution methods, since the convolution input (kernel) functions meet the basic requirements defined in Anderson (1982, p. 346) and Anderson (1979, p. 1289). Equations (10)–(11) have increasing (unbounded) kernels, and would certainly fail for any argument value if used directly in ZHANKS or DHANKL. Algebraically divergent integrals can often be converted to convergent form using transformations as previously mentioned; however, I will not consider (10)–(11) any further.

To illustrate the above discussion, subprogram DHANKL (Anderson, 1982) was run on a VAX-11/780 VMS/3.5 system in double-precision complex arithmetic (COMPLEX*16) for the same examples presented in Chave's Table 2. The divergent types (10)–(11) were excluded, as well as the oscillating types (12)–(13) for argument $R = 0.05$. My DHANKL results are listed in Table I.

The tolerance factor (TOL) used in Table I was selected the same as parameter RERR in Chave's Table 2. The number of kernel function evaluations used in DHANKL for direct convolution is denoted by NF in Table I, and $NF = 0$ denotes related convolution was used. Note that the accuracy in NUMERR for oscillatory integrals $NN = 7$ and $NN = 8$ at $R = 2.0$ is only good to about three figures; however, these same integrals at $R = 100.0$ are nearly equivalent to those in Chave's Table 2. All remaining results in Table I clearly show comparable accuracy with Chave's Table 2 and with respect to the computed exact values and requested accuracy (see TOL in Anderson, 1982, p. 352 and double-precision version, p. 364).

It is stated on p. 1674 that "Table 2 shows similar computations [as in Table I] with RERR = 10^{-10}, a far more stringent requirement with a concomitant increase in compu-

Table I. VAX-11/780 results using double-precision DHANKL (Anderson, 1982).

NN	R	TOL	NUMERR	NUMERI	EXACTR	EXACTI	NF
1	0.05	0.1D-09	0.3535533216	-0.3532409598	0.3535533216	-0.3532409596	340
2	0.05	0.1D-09	0.2495322253E-01	0.0000000000E+00	0.2495322244E-01	0.0000000000E+00	236
3	0.05	0.1D-09	19.99999999	0.0000000000E+00	20.00000000	0.0000000000E+00	719
4	0.05	0.1D-09	19.29318260	-0.6824013725	19.29318268	-0.6824013726	478
1	2.00	0.1D-09	0.2457792119	-0.1928177160E-01	0.2457791604	-0.1928180249E-01	157
2	2.00	0.1D-09	0.2763932020	0.0000000000E+00	0.2763932023	0.0000000000E+00	156
3	2.00	0.1D-09	0.4999999998	0.0000000000E+00	0.5000000000	0.0000000000E+00	719
4	2.00	0.1D-09	0.1895626027E-01	-0.1200712143	0.1895626091E-01	-0.1200712156	470
7	2.00	0.1D-09	0.4992191583	0.0000000000E+00	0.5000000000	0.0000000000E+00	394
8	2.00	0.1D-09	0.8659400089	0.0000000000E+00	0.8660254038	0.0000000000E+00	0
1	100.00	0.1D-09	-0.9963758581E-11	0.6355519647E-12	0.0000000000E+00	0.0000000000E+00	158
2	100.00	0.1D-09	0.9900004998E-02	0.0000000000E+00	0.9900005000E-02	0.0000000000E+00	180
3	100.00	0.1D-09	0.9999999997E-02	0.0000000000E+00	0.1000000000E-01	0.0000000000E+00	719
4	100.00	0.1D-09	-0.4365570173E-11	0.1988721242E-12	-0.4851871203E-34	-0.1952579141E-32	487
7	100.00	0.1D-09	0.9999804157E-02	0.0000000000E+00	0.1000000000E-01	0.0000000000E+00	391
8	100.00	0.1D-09	0.9999499931	0.0000000000E+00	0.9999499987	0.0000000000E+00	0

tational overhead." Of course this is the price paid for double-precision accuracy, but it also includes the cost of computing more Bessel functions, as required by direct quadrature methods. To compare computer processing unit (CPU) times fairly between direct quadrature and convolution methods, I reproduced Chave's Tables 1 and 2 (using his published program and IMSL Bessel function subprograms), excluding the same lines as in my Table I, and reran DHANKL using TOL = .1D-5. For brevity, the latter results are not given, but commensurate accuracy was obtained as in Chave's Table 1. Total VAX execution CPU times (seconds) for all integration subprograms in each table, excluding most of the driver and all I/0-times, plus total functions calls (Sum NF), are summarized in Table II.

Table II shows, for equal tolerances, that the direct quadrature method requires significantly more computer time than convolution, rather than "slightly more" as stated on page 1674. The single-precision convolution routines HANKEL and ZHANKS were also run, yielding results of lower accuracy (about four–five figures) than those obtained from DHANKL, but execution times were much smaller. The tabulated computational speed variations would be quite important in programs needing many hundreds or thousands of Hankel transforms, such as in one-dimensional inversion of EM sounding data over layered media, or in three-dimensional EM integral equation modeling.

Chave's direct quadrature algorithm is an important complement to the digital filter method, especially when double-precision Hankel transforms are needed which contain difficult kernels or extreme argument ranges. A hybrid procedure that exploits the best features of both algorithms—thereby obtaining an efficient and accurate method suitable to a larger class of problems—would be a valuable future contribution.

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REFERENCES

Anderson, W. L., 1979, Numerical integration of related Hankel transforms of orders 0 and 1 by adaptive digital filtering: Geophysics, **44**, 1287–1305.

——— 1982, Fast Hankel transforms using related and lagged convolutions: ACM Trans. on Math. Software, **8**, 344–368.

Frischknecht, F. C., 1967, Fields about an oscillating magnetic dipole over a two-layer earth and application to ground and airborne electromagnetic surveys: Quart. Colo. School of Mines, **62**, no. 1, 326 p.

Table II. Comparison of VAX-11/780 total CPU times (s).

Table no.	TOL or RERR	Quadrature time	Quadrature Sum(NF)	DHANKL..... time	DHANKL..... Sum(NF)	HANKEL or ZHANKS time	HANKEL or ZHANKS Sum(NF)
* 1	.1E-5	4.54	3649	1.68	3254	.42	1365
* 2	.1E-9	9.59	7646				
I	.1D-9			2.66	5604		

* Tables 1 and 2 had same lines excluded as in Table I above.

Reply by the author to W. L. Anderson

Anderson presents an interesting comparison of my direct quadrature Hankel transform algorithm with a high precision (~ 12 significant figures) digital filter procedure that he published recently. His clarifications regarding lagged convolution are important. However, two of his major points may be misleading, and require a more careful examination.

From Anderson's Table II, one would conclude that the direct quadrature algorithm generally requires more kernel function evaluations, and hence a higher computational burden, than the digital filter method. A more careful examination of my Table 2 and Anderson's Table I shows that this is quite problem dependent, and both algorithms display marked advantages for specific combinations of the functional form of the kernel and the range parameter. A thorough comparison of the two algorithms would include the cost of computing the Bessel functions for the direct quadrature case, and this is dependent on the method used to obtain them, which Anderson does not specify. Finally, the amount of CPU time required for a numerical procedure is hardware dependent, especially with the advent of vector pipeline architecture (e.g., CRAY). My conclusion is that the relative advantages of the two algorithms, assuming that computer usage is the predominant criterion, should be evaluated for any problem of interest to the user.

My second comment concerns the statements that Anderson makes concerning transformations of the kernel function so that standard numerical quadrature, or the digital filter algorithm, will work on formally divergent integrals. These methods often work, although care is usually required to avoid loss of significance because the transformed numerical result and the analytic term that is added to it often have similar magnitudes and opposite signs. In some cases, it is quite difficult to determine the proper asymptotic form of the kernel; an example occurs for the Frechet derivatives of electromagnetic induction that are required for Backus-Gilbert inversion of field data. Finally, except in those cases where computer usage is an overwhelming consideration, the labor involved in correctly applying kernel transformations may not be worthwhile.

The direct quadrature algorithm was not intended as a replacement for the digital filter method, but was offered as an alternate way to solve difficult problems. I agree with Anderson that a hybrid approach is probably best; this is the manner in which I have solved sea floor controlled source problems. I am grateful to Anderson for his comments, and for the valuable contributions he has made to the solution of electromagnetic induction problems.

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