JOURNAL OF COMPUTATIONAL PHYSICS **11**, 28–37 (1973)

The Accurate Calculation of Fourier Integrals by the Fast Fourier Transform Technique

FLAVIAN ABRAMOVICI

Department of Mathematical Sciences, Tel Aviv University, Ramat Aviv, Tel Aviv, Israel

Received November 30, 1971

It is shown how simple integration rules can be associated with the Fast Fourier Transform technique in order to obtain accurate results without reducing essentially the speed of computation. The results of several numerical experiments are presented.

1. INTRODUCTION

Due to the widespread use of the Fourier Transform, it is very important to have methods for numerical calculation, that are both fast and accurate. In practice we do not compute the infinite Transform of a time-function $f(t)$ but the Finite Transform

$$\Phi(\omega) = \int_0^T f(t)\, e^{-i\omega t}\, dt, \tag{1}$$

the function $f(t)$ being known only at a finite number of equidistant points

$$t_j = j\,\Delta t = jT/N, \qquad j = 0, 1,..., N-1. \tag{2}$$

When $\phi(\omega)$ is wanted at a large number of equally spaced points, the computing-time of (1) is tremendously reduced by using the Fast Fourier Transform technique (F.F.T.) proposed by Cooley and Tukey [1]. The integral (1) is approximated by

$$\Phi_1(\omega) = (T/N) \sum_{j=0}^{N-1} f(t_j)\, e^{-i\omega t_j}, \tag{3}$$

and calculated for the following values of ω:

$$\omega_k = k\,\Delta\omega = k(2\pi/T), \qquad k = 0, 1,..., N-1, \tag{4}$$

N being a power of 2. When the data are noisy, e.g., when working with rounded numbers, the F.F.T. gives a total error smaller than when summing directly, the improvement ratio being proportional to $N/\log N$ [2].

The numerical integration rule represented by (3) is a very crude one, the truncation error E being proportional to $\Delta t = T/N$. As it has been shown by Cooley, Lewis and Welch [3], if the function $f(t)$ has additional properties the order of the method is higher; e.g., if $f(0) = f(T)$ (3) becomes the usual trapezoidal rule so that $E = O((\Delta t)^2)$ or if the odd-order derivatives $f'(t), f'''(t),..., f^{(2k-1)}(t)$ are equal at the end-points 0 and T, then (3) is equivalent to the trapezoidal rule with end corrections and $E = O((\Delta t)^{2k+1})$.

If the function $f(t)$ has none of these properties and one needs a better accuracy, one uses a higher order numerical quadrature formula, the classical one for this type of integral being that proposed by Filon [4], with a truncation error $E = O((\Delta t)^3)$.

It seems therefore that, except in particular cases, either one can compute the Finite Transform very fast but then the accuracy is low, or else one obtains higher accuracy but then the speed is drastically reduced. Mandel and Bearman [5] proposed methods to reconciliate speed and accuracy by associating the F.F.T. with a modification of an integration formula based on the trapezoidal rule and also with Filon's method. They also compared the accuracy of the results obtained by using these techniques.

In the present paper we show with illustrative examples how known numerical techniques associated with the F.F.T. give very accurate results without reducing essentially the computational speed.

2. The F.F.T. and Integration Rules with Equidistant Nodes

As has been mentioned previously, if $f(0) = f(T)$, (3) is equivalent to the trapezoidal rule, as for the values (4) of ω, the integrand of (1),

$$F(t) = f(t)\, e^{-i\omega t}, \tag{5}$$

has equal values at the end-points of the integration interval $t_0 = 0$ and $t_N = T$, so that

$$\Phi_1(\omega) = \Delta t \sum_{j=0}^{N-1} F(t_j) = \Delta t \left\{ 1/2[F(t_0) + F(t_N)] + \sum_{j=1}^{N-1} F(t_j) \right\}. \tag{6}$$

In fact, the imaginary part of the integrand has equal values at the end-points even if $f(t)$ does not, and this explains why the F.F.T. gives more accurate results for the imaginary part of the Transform $\Phi_I = -\int_0^T f(t) \sin \omega t \, dt$, than for the real part $\Phi_R = \int_0^T f(t) \cos \omega \, dt$.

Suppose that we know the value of $f(t)$ for $t = t_N$. Then, the auxiliary function

$$g(t) = f(t) - \frac{f(T) - f(0)}{T} t - f(0) \tag{7}$$

obtained from $f(t)$ by removal of a linear trend has equal values at the end-points so that the real part of the transform $\Psi(\omega) = \int_0^T g(t)\, e^{-i\omega t}\, dt$ will be calculated by the F.F.T. according to the trapezoidal rule. Lanczos [6] proposed the removal of the linear trend in order to improve the convergence of the Fourier series of $f(t)$. As it turns out, this operation has an improving effect also on the accuracy of the Fourier coefficients. The imaginary part will be calculated even with a better accuracy, as the corresponding integrand $G(t) = g(t) \sin \omega t$ satisfies also the condition $G'(0) = G'(T)$. The Fourier Transform $\Phi(\omega)$ will be then obtained from

$$\Phi(\omega) = \Psi(\omega) - \frac{1}{T\omega} \Big\{ f(T) \left[\frac{1}{\omega} - e^{-i\omega T} \left(\frac{1}{\omega} - iT \right) \right] - f(0) \left[\frac{1}{\omega} - \frac{e^{-i\omega T}}{\omega} + iT \right] \Big\}. \tag{8}$$

By using this procedure (let us call it "trapezoidal F.F.T.") we improve accuracy without reducing essentially the speed of calculation, the number of additional arithmetic operations needed being proportional to the number of integration points N. It may happen in practice that the trapezoidal F.F.T. even reduces the number of operations as it gives a much better accuracy with a smaller number of integration points.

In order to associate the F.F.T. technique with higher-order integration formulas we introduce the auxiliary function

$$h(t_j) = \alpha_j g(t_j), \tag{9}$$

where α_j are proportional to the weights of some integration rule with equidistant nodes for calculating $\Psi(\omega)$

$$\Psi(\omega) = \int_0^T g(t)\, e^{-i\omega t}\, dt \simeq \sum_{j=0}^{N-1} \alpha_j g(t_j)\, e^{-i\omega t_j} = \sum_{j=0}^{N-1} h(t_j)\, e^{-i\omega t_j}. \tag{10}$$

The last sum is of the form (3) and the F.F.T. can be applied.

We experimented with two composite integration rules based on higher-order closed Newton–Cotes formulas: the Simpson rule and the 5-points rule

$$\int_{x_0}^{x_4} f(x)\, dx \simeq \frac{2h}{45} (7f_0 + 32f_1 + 12f_2 + 32f_3 + 7f_4), \tag{11}$$

the truncation error being $O(h^4)$ and $O(h^6)$, respectively. The results shown illustrate the known fact that the Newton–Cotes formulas are less accurate when large numbers of points are used and should be avoided.

TABLE I

Values of $\phi_I(\omega) = \int_0^T f(t) \sin \omega t \, dt$ for $f(t) = t \cos \omega_0 t$, $\omega_0 = 1$, $T = 2\pi$

ω	Exact value	No. of integr. points	F.F.T.	Filon	Trapezoidal F.F.T.	Simpson F.F.T.	5-points F.F.T.
1	-1.57079632679						
		64	$-1.56\|574647944$	$-1.5707\|6154092$	$-1.57079\|388481$	$-1.570\|80610140$	$-1.570796\|13415$
		256	$-1.570\|48090016$	$-1.570796\|19068$	$-1.5707963\|1548$	$-1.5707963\|6240$	$-1.57079632\|549$
		1024	$-1.5707\|7661299$	$-1.5707963267\|0$	$-1.570796326\|27$	$-1.570796326\|30$	$-1.570796326\|11$
		2048	$-1.57079\|139819$	$-1.57079632\|804$	$-1.570796326\|52$	$-1.570796326\|45$	$-1.570796326\|42$
30	$-2.09672479661 \times 10^{-1}$						
		64	-3.04512513772×10	$1.78252346600 \times 10^{-1}$	$-2.09\|513536990 \times 10^{-1}$	$-5.58577760443 \times 10^{-1}$	$-6.51689060446 \times 10^{-1}$
		256	$-2.0\|0123197561 \times 10^{-1}$	$-2.0\|4609246414 \times 10^{-1}$	$-2.09672\|182030 \times 10^{-1}$	$-2.0967\|3897498 \times 10^{-1}$	$-2.096724\|65355 \times 10^{-1}$
		1024	$-2.09\|080746494 \times 10^{-1}$	$-2.096\|51207669 \times 10^{-1}$	$-2.0967247\|8545 \times 10^{-1}$	$-2.096724\|84175 \times 10^{-1}$	$-2.09672479\|462 \times 10^{-1}$
		2048	$-2.09\|524609265 \times 10^{-1}$	$-2.0967\|1145328 \times 10^{-1}$	$-2.09672479\|591 \times 10^{-1}$	$-2.09672479\|940 \times 10^{-1}$	$-2.096724796\|58 \times 10^{-1}$
100	$-6.2838136885 \times 10^{-2}$						
		256	$-2.75937570533 \times 10^{-2}$	$-2.09264373658 \times 10^{-2}$	$6.283\|65404236 \times 10^{-2}$	$-6.2\|9319781354 \times 10^{-2}$	$6.283\|23530407 \times 10^{-2}$
		1024	$-6.\|08543252165 \times 10^{-2}$	$-6.2\|0879894257 \times 10^{-2}$	$6.283813\|30614 \times 10^{-2}$	$-6.28381\|541443 \times 10^{-2}$	$-6.28381\|257799 \times 10^{-2}$
		2048	$-6.2\|3445302997 \times 10^{-2}$	$6.2\|7893183552 \times 10^{-2}$	$-6.2838136\|6518 \times 10^{-2}$	$-6.283813\|78486 \times 10^{-2}$	$-6.2838136\|7622 \times 10^{-2}$
500	$-1.2566420880 \times 10^{-2}$						
		1024	$-7.10004847431 \times 10^{-1}$	$1.19364113290 \times 10^{-2}$	$-1.2566\|3773062 \times 10^{-2}$	$-1.\|37868871242 \times 10^{-2}$	$-1.\|411235880127 \times 10^{-2}$
		2048	$-9.99986896475 \times 10^{-3}$	$-8.16351380408 \times 10^{-3}$	$-1.256641\|94740 \times 10^{-2}$	$-1.25664\|335300 \times 10^{-2}$	$-1.24\|8506995702 \times 10^{-2}$

TABLE II

Values of $\phi_l(\omega) = \int_0^T f(t) \sin \omega t$ for $f(t) = t \cos \omega_0 t$, $\omega_0 = 50$, $T = 2\pi$

ω	Exact values	No. of integr. point	F.F.T.	Filon	Trapezoidal F.F.T.	Simpson F.F.T.	5-points F.F.T.
1	$2.51427983481 \times 10^{-3}$						
		256	$2.85494470456 \times 10^{-3}$	$2.38324116952 \times 10^{-3}$	$2.53952938240 \times 10^{-3}$	$2.38303882862 \times 10^{-3}$	$3.00192628782 \times 10^{-3}$
		1024	$2.53408622951 \times 10^{-3}$	$2.51390235564 \times 10^{-3}$	$2.51437295245 \times 10^{-3}$	$2.51390169916 \times 10^{-3}$	$2.51430364634 \times 10^{-3}$
		2048	$2.51921395392 \times 10^{-3}$	$2.51425657545 \times 10^{-3}$	$2.51428563348 \times 10^{-3}$	$2.51425652726 \times 10^{-3}$	$2.51428018254 \times 10^{-3}$
30	$1.17809724510 \times 10^{-1}$						
		256	$1.28152385161 \times 10^{-1}$	$1.17260100921 \times 10^{-1}$	$1.18603400691 \times 10^{-1}$	$1.12503860903 \times 10^{-1}$	$1.02718754065 \times 10^{-1}$
		1024	$1.18404257787 \times 10^{-1}$	$1.17813448863 \times 10^{-1}$	$1.17812525735 \times 10^{-1}$	$1.17798224568 \times 10^{-1}$	$1.17811032511 \times 10^{-1}$
		2048	$1.17957769079 \times 10^{-1}$	$1.17809969324 \times 10^{-1}$	$1.17809898743 \times 10^{-1}$	$1.17809023079 \times 10^{-1}$	$1.17809742980 \times 10^{-1}$
100	$-8.37758040957 \times 10^{-2}$						
		256	$4.40721645739 \times 10^{-2}$	$1.34031587053 \times 10^{-2}$	$-7.93149479442 \times 10^{-2}$	$2.99045844469 \times 10^{-2}$	$6.76580673335 \times 10^{-2}$
		1024	$-8.17823988792 \times 10^{-2}$	$8.30145505882 \times 10^{-2}$	$-8.37662067240 \times 10^{-2}$	$8.38198803076 \times 10^{-2}$	$8.37388546403 \times 10^{-2}$
		2048	$-8.32816129992 \times 10^{-2}$	$-8.37262311114 \times 10^{-2}$	$8.37752193513 \times 10^{-2}$	$8.37782235605 \times 10^{-2}$	$-8.37754464441 \times 10^{-2}$
500	$-1.26933036509 \times 10^{-2}$						
		1024	$-7.26994302608 \times 10^{-4}$	$1.19363225189 \times 10^{-2}$	$1.25833667614 \times 10^{-2}$	$1.72617478298 \times 10^{-1}$	$2.21997989818 \times 10^{-1}$
		2048	$1.01232340181 \times 10^{-2}$	$8.29041794084 \times 10^{-3}$	$1.26897845274 \times 10^{-2}$	$1.27252571161 \times 10^{-2}$	$2.50814394771 \times 10^{-2}$

TABLE III

Values of $\phi_R = \int_0^T f(t) \cos \omega t$ for $f(t) = t \cos \omega_0 t$ $\omega_0 = 50$ $T = 2\pi$

ω	Exact value	No. of integr. point	F.F.T.	Filon	Trapezoidal F.F.T.	Simpson F.F.T.	5-point F.F.T.
10.	0.						
		256	-7.7×10^{-2}	3.2×10^{-14}	-1.2×10^{-9}	-1.6×10^{-9}	-1.7×10^{-9}
		1024	-1.9×10^{-2}	1.7×10^{-12}	-3.4×10^{-10}	-4.4×10^{-10}	-4.7×10^{-10}
		2048	-9.6×10^{-3}	2.2×10^{-12}	-2.1×10^{-10}	-2.6×10^{-10}	-2.7×10^{-10}
50.	9.86960440109						
		256	9.|79249811782	9.|55018882140	9.86960440|072	9.86960440|588	9.86960440|055
		1024	9.8|5032783007	9.86|816118692	9.86960440|088	9.86960440|081	9.86960440|079
		2048	9.8|5996611559	9.869|51354085	9.86960440|099	9.86960440|095	9.86960440|094

3. Numerical Results

Values of the imaginary part of the Transform $\Phi_I(\omega)$ as calculated by using the methods described previously and compared with those given by Filon's method, the usual F.F.T. and the exact ones for the function $f(t) = t \cos \omega_0 t$, are shown in Tables I and II. This function was considered for illustrating numerical integration procedures by Davis and Rabinowitz [7]. In Table I, $\omega_0 = 1$, while in Table II, $\omega_0 = 50$. In Table III are shown values of the real part of the Transform $\Phi_R(\omega)$ for the same function, for $\omega_0 = 50$. The vertical lines within the numbers appearing in the tables mark the end of the string of digits that coincide with those in the exact solution.

Although the numbers shown in the tables speak for themselves, we want to stress the following general points.

For moderate values of ω, the trapezoidal F.F.T. is almost as accurate as Filon, while higher order composite formulas associated with the F.F.T. are more accurate, as it should be. For large values of ω or for a very oscillatory integrand, the Filon's method (even for $\theta = \omega \, \Delta t < 1$) as well as the higher-order methods are so inaccurate that even the order of magnitude of the result is wrong so that the only method to be used seems to be the trapezoidal F.F.T. The results for large ω calculated by using Filon's method are given only for the sake of comparison, as this method is most accurate and useful when $f(t)$ is a reasonably smooth function.

4. The Romberg Integration

Computing the Fourier Transform $\Psi(\omega)$ of $g(t)$ instead of $f(t)$ has an additional advantage: One can improve the accuracy by using the Romberg procedure, i.e., by building the sequence

$$I_{N_j}^{(k+1)} = (4^{k_0+k} I_{N_j}^{(k)} - I_{N_{j-1}}^{(k)})/(4^{k_0+k} - 1) \tag{12}$$

for several values of k, where $I_{N_j}^{(0)}$ is the result given either by the simple trapezoidal rule or by the trapezoidal rule with end-corrections with N_j integration points and

$$N_{j+1} = 2N_j \, . \tag{13}$$

For illustration, we give in Table IV some values of the imaginary part of the Transform for $f(t) = t \cos \omega_0 t$ with $\omega_0 = 50$. Here we have to take $k_0 = 1$. In Table V are given the values of the real and imaginary parts of the Transform for the function $f(t) = e^{\alpha t} \sin \beta t$ for $\alpha = 0.1$, $\beta = 0.5$. For the real part of the Transform, $k_0 = 0$, and for the imaginary part, $k_0 = 1$.

TABLE IV

Values of $\phi_I(\omega) = \int_0^T f(t) \sin \omega t \, dt$ for $f(t) = t \cos \omega_0 t$, $\omega_0 = 50$, $T = 2\pi$[a]

ω	Exact value	No. of integr. points	$k = 0$	$k = 1$	$k = 2$	$k = 3$	$k = 4$
1	$2.51427983481 \times 10^{-3}$						
		256	$2.5\vert 3952938240 \times 10^{-3}$				
		512	$2.51\vert 578671728 \times 10^{-3}$	$2.5142\vert 0387294 \times 10^{-3}$			
		1024	$2.514\vert 37295245 \times 10^{-3}$	$2.51427\vert 870146 \times 10^{-3}$	$2.5142798\vert 8921 \times 10^{-3}$		
30	$1.17809724510 \times 10^{-1}$						
		256	$1.1\vert 0597510251 \times 10^{-1}$				
		512	$1.178\vert 55429237 \times 10^{-1}$	$1.1780\vert 5564474 \times 10^{-1}$			
		1024	$1.178\vert 12525735 \times 10^{-1}$	$1.17809\vert 665502 \times 10^{-1}$	$1.178097\vert 30598 \times 10^{-1}$		
		2048	$1.17809\vert 898743 \times 10^{-1}$	$1.1780972\vert 3610 \times 10^{-1}$	$1.178097245\vert 33 \times 10^{-1}$	$1.1780972450\vert 9 \times 10^{-1}$	
100	$-8.37758040957 \times 10^{-2}$						
		256	$-7.93149479442 \times 10^{-2}$				
		512	$-8.3\vert 6051859726 \times 10^{-2}$	$-8.3\vert 8912018411 \times 10^{-2}$			
		1024	$-8.37\vert 662067240 \times 10^{-2}$	$-8.377\vert 69414408 \times 10^{-2}$	$-8.3775\vert 1277836 \times 10^{-2}$		
		2048	$-8.3775\vert 2193513 \times 10^{-2}$	$-8.37758\vert 201931 \times 10^{-2}$	$8.377580\vert 23955 \times 10^{-2}$	$-8.377580\vert 50410 \times 10^{-2}$	
		4096	$-8.3775\vert 7677796 \times 10^{-2}$	$-8.3775804\vert 3415 \times 10^{-2}$	$8.37758040\vert 899 \times 10^{-2}$	$-8.377580409\vert 65 \times 10^{-2}$	$-8.3775804095\vert 6 \times 10^{-2}$

[a] As calculated by the Romberg procedure. $k_0 = 1$.

TABLE V

Values of $\phi_R(\omega) = \int_0^T f(t) \cos \omega t \, dt$ and $\phi_I(\omega) = \int_0^T f(t) \sin \omega t \, dt$ for $f(t) = e^{\alpha t} \sin \beta t$[a]

Function	k_0	ω	Exact value	No. of integr. points	$k = 0$	$k = 1$	$k = 2$
$\phi_R(\omega)$	0	$2\pi/10$	-1.09725568604				
				256	$-1.097\|30815623$		
				512	$-1.0972\|6881085$	$-1.0972556960\|8$	
				1024	$-1.09725\|897477$	$-1.0972556960\|8$	$-1.0972556960\|7$
		12π	$-2.90311478993 \times 10^{-4}$				
				256	$-3.48987354373 \times 10^{-4}$		
				512	$-3.03789292224 \times 10^{-4}$	$-2.90\|220160261 \times 10^{-4}$	
				1024	$-2.9\|3612443252 \times 10^{-4}$	$-2.903\|05886465 \times 10^{-4}$	$-2.90311\|601545 \times 10^{-4}$
				2048	$-2.9\|1132525662 \times 10^{-4}$	$-2.90311\|131245 \times 10^{-4}$	$-2.903114\|80897 \times 10^{-4}$
$\phi_I(\omega)$	1	$2\pi/10$	2.66749577010				
				256	$2.6674957\|6884$		
				512	$2.6674957\|6994$	$2.667495770\|06$	
				1024	$2.667495770\|05$	$2.667495770\|08$	$2.667495770\|08$
		12π	$9.36072839917 \times 10^{-3}$				
				256	$9.360\|65233224 \times 10^{-3}$		
				512	$9.36072\|423884 \times 10^{-3}$	$9.360728\|40736 \times 10^{-3}$	
				1024	$9.360728\|14683 \times 10^{-3}$	$9.36072839\|894 \times 10^{-3}$	$9.36072839\|881 \times 10^{-3}$
				2056	$9.3607283\|8319 \times 10^{-3}$	$9.360728399\|03 \times 10^{-3}$	$9.3607283399\|0 \times 10^{-3}$

[a] $\alpha = 0.1$, $\beta = 0.5$, as calculated by the Romberg procedure.

Acknowledgments

The numerical work related to the paper has been performed on the CDC 6600-Computer of the Tel Aviv University, and I am grateful to Professor Amnon Jakimovski, Head of the Department of Mathematical Sciences, for allowing me the necessary computing time. I would also like to thank Mrs. Shula Finkelstein for the programming related to the numerical results presented here. Part of the work has been supported by a grant given by the Natural Sciences Department of the Tel Aviv University.

References

1. J. W. Cooley and J. W. Tukey, *Math. Comput.* **19** (1965), 297.
2. T. Kaneko and B. Liu, *J. Assoc. Comp. Mach.* **17** (1970), 637.
3. J. W. Cooley, P. A. W. Lewis and P. D. Welch, *IEEE Trans. Audio Electroacoust.* **AU-15** (1967), 79.
4. L. N. G. Filon, *Proc. Roy. Soc. Edinburgh* **49** (1928), 38.
5. F. Mandel and R. J. Bearman, *J. Comput. Phys.* **7** (1971), 637.
6. C. Lanczos, "Applied Analysis," Prentice-Hall, Englewood Cliffs, NJ 1956.
7. P. S. Davis and P. Rabinowitz, "Numerical Integration," Blaisdell, Waltham, MA, 1967.