Mathematics Notes

Note 37

August 1974

SUBROUTINE CAUCHY: COMPLEX ROOTS OF A FUNCTION USING A CAUCHY INTEGRAL TECHNIQUE

C. O. Beasley, Jr. and H. K. Meier Oak Ridge National Laboratory, Oak Ridge, Tennessee

ABSTRACT

A description of the subroutine CAUCHY, the program for finding zeros of an analytic function f(z) within a contour in the z-plane, is given. Examples of types of functions for which this program is most advantageous as well as types of functions which show its weaknesses, are given.

ACKNOWLEDGEMENT

Research sponsored by U. S. Atomic Energy Commission under contract with Union Carbide Corporation.

I. Introduction

The purpose of this report is to describe in detail the sub-routine CAUCHY and its subprograms. This routine is used to find the zeros of an arbitrary function f(z) within a contour c in the complex z-plane.

The method used has been documented. It relies on calculating integrals of the form

$$S_{N} = \frac{1}{2\pi i} \oint z^{N} \frac{f'(z)}{f(z)} dz = \sum_{i=1}^{M} z_{i}^{N} - \sum_{j=1}^{K} w_{i}^{N}$$
(1)

where z_i are the zeros and w_i are the poles of f within c. Thus if there are no poles, S_0 gives the number of zeros, S_1 the sum of the zeros, S_2 the sum of their squares, etc.

This method becomes numerically practical when c contains a small number of zeros. Thus some knowledge of f is desirable, and in principle, if sufficiently small integration steps are taken so that the function is sufficiently smooth, the answer may be obtained to arbitrary accuracy. Since the method does not rely on iteration, it will work even when well-known iteration methods will not.

The problem is then to perform the integral with suitable accuracy. One straight-forward method is found in the programs ISQNK1 and ISQNK2 from the Massachusetts Institute of Technology Information Processing Center. The method used by these programs is to integrate (1) by parts, and then use a Simpson's rule integration to perform the numerical integration around c. The program is most useful when large numbers of points of c may be calculated and when a large number of roots may exist ($M \le 4$ for this program). An automatic increasing or decreasing of step size along c is included in the program.

In many cases of numerical interest, it is costly to compute the function, and one would like to locate one or two zeros with fair accuracy with a minimum number of points. The presence of nearby poles or zeros in f introduces poles on the integrand of equation 1 and may make normal integration procedures impractical because of the large number of contour points required. It is these cases for which the subroutine CAUCHY is designed.

In the next section, we will discuss the method. In the third section, we describe the subroutines. The fourth section gives some sample results, and the fifth a listing of the subroutine and its subprograms

II. METHOD

Suppose we are given three values of a function \mathbf{f}_j at three points \mathbf{z}_j . We can form a best-fit binomial

$$f_{approx} = a z^2 + b z + c$$
 (2)

by determining a, b, and c. Now we may factor f approx

$$f_{approx} = (z - z_1)(z - z_2)$$
 (3)

where

$$z_{1,2} = -\frac{b \pm \sqrt{b^2 - 4 a c}}{2a}$$

Then

$$f'_{approx} = (z - z_2) + (z - z_1)$$

and

$$\frac{f'_{approx}}{f_{approx}} = \frac{1}{z - z_1} + \frac{1}{z - z_2} \tag{4}$$

So we may perform our integral over the segment of the contour c over which (2) is valid; the integrals are of the form

$$\int_{z_{a}}^{z_{b}} dz \frac{z^{n}}{z-z_{\alpha}} \qquad n = 0,1,2 \dots$$

$$= \mathcal{M}\left(\frac{z_{b}-z_{\alpha}}{z_{a}-z_{\alpha}}\right) \qquad n = 0$$

$$= (z_{b}-z_{a}) - \mathcal{M}\left(\frac{z_{b}-z_{\alpha}}{z_{a}-z_{\alpha}}\right) \qquad n = 1$$

$$= \frac{1}{2} (z_{b}-z_{a})(z_{b}+z_{a}-2z_{\alpha}) - 2(z_{b}-z_{a}) + \mathcal{M}\left(\frac{z_{b}-z_{\alpha}}{z_{a}-z_{\alpha}}\right) \qquad n = 2$$

However, (2) is not a good approximation to f if f has nearby singularities. A much better approximation obtains if f_j is known at five points z_j :

$$f_{approx} = \frac{c_1 + c_2 z + c_3 z^2}{c_4 + c_5 z + c_6 z^2}$$
 (6)

We may factor both numerator and denominator

$$f_{approx} = \frac{(z-z_{n1})(z-z_{n2})}{(z-z_{d1})(z-z_{d2})} \frac{c_3}{c_6}$$
 (7)

So

$$\frac{f'_{approx}}{f_{approx}} = \frac{1}{z - z_{nl}} + \frac{1}{z - z_{n2}} - \frac{1}{z - z_{dl}} - \frac{1}{z - z_{d2}}$$
(8)

Thus in calculating the integral (5), one adds the contributions from the roots of the numerator and subtracts those of the denominator.

We must first solve for the c_i . We can make the numerical computation more accurate by transforming to a coordinate system where the center point of the five z_j , z_o , is zero; thus we know our function at five points f_{-2} , f_{-1} , f_o , f_1 , and f_2 . We can then write (6) as

$$c_1 + c_2 z_j + c_3 z_j^2 = (c_4 + c_5 z_j + c_6 z_j^2) f_j$$
 (9)

We note that (9) is a set of five linear equations for the six c_i . We may write the c_i as follows. We first note that at $z_0 = 0$,

$$c_1 = c_4 f_0 \tag{10}$$

Using this, we may write the other numerator coefficients c_2 and c_3 in terms of the denominator coefficients:

$$c_{2} = \frac{z_{1} z_{-1} (f_{-1} - f_{1})}{z_{1} - z_{-1}} c_{6} + \frac{(z_{1} f_{-1} - z_{-1} f_{1})}{z_{1} - z_{-1}} c_{5} + (11)$$

$$+ \frac{1}{z_{1} - z_{-1}} \left[\frac{z_{1}}{z_{-1}} (f_{-1} - f_{0}) - \frac{z_{-1}}{z_{1}} (f_{1} - f_{0}) \right] c_{4}$$

$$c_{3} = \frac{z_{1}f_{1} - z_{-1}f_{-1}}{z_{1} - z_{-1}} c_{6} + \frac{f_{1} - f_{-1}}{z_{1} - z_{-1}} c_{5} + \frac{1}{z_{1} - z_{-1}} \left[\frac{f_{1} - f_{0}}{z_{1}} - \frac{f_{-1} - f_{0}}{z_{-1}} \right] c_{4}$$
(12)

If we put c_1 , c_2 , and c_3 in (9) and divide by z_1 ,

$$A^{j} c_{5} + B^{j} c_{6} = C^{j} c_{4} \quad (j = \pm 2)$$
 (13)

where

$$A^{j} = \frac{z_{j} (f_{1} - f_{-1})}{z_{1} - z_{-1}} + \frac{(z_{1} f_{-1} - z_{-1} f_{1})}{z_{1} - z_{-1}} - f_{j}$$
 (14)

$$B^{j} = \frac{z_{j}(z_{1}f_{1}-z_{-1}f_{-1})}{z_{1}-z_{-1}} + \frac{z_{1}z_{-1}(f_{-1}-f_{1})}{z_{1}-z_{-1}} - z_{j}f_{j}$$
 (15)

$$C^{j} = \frac{f_{j}^{-f} \circ}{z_{j}} - \frac{1}{z_{1}^{-z} - 1} \left[\frac{z_{1}}{z_{-1}} \left(f_{-1} - f_{0} \right) - \frac{z_{-1}}{z_{1}} \left(f_{1}^{-f} - f_{0} \right) \right] - \frac{z_{j}^{-1}}{z_{1}^{-z} - 1} \left[\frac{f_{1}^{-f} \circ}{z_{1}} - \frac{f_{-1}^{-f} \circ \circ}{z_{-1}} \right]$$
(16)

 $A^{j} = B^{j} = C^{j} = 0$ for $j = 0, \pm 1$. We now solve (13) for c_{5} and c_{6} :

$$c_{5} = \frac{c_{4}}{DET} \begin{pmatrix} c^{2} & B^{2} \\ c^{-2} & B^{-2} \end{pmatrix}$$
 (17)

$$c_6 = \frac{c_{1_4}}{DET} \begin{vmatrix} A^2 & c^2 \\ A^{-2} & c^{-2} \end{vmatrix}$$
 (18)

where

$$DET = A^2 B^{-2} - B^2 A^{-2}$$
 (19)

If we now set c_{\downarrow} = DET, we have a unique solution for the c_{\downarrow} .

Problems do arise if DET = 0. This will happen when f is of the form

$$f = \frac{\alpha_0 + \alpha_1 z}{\beta_0 + \beta_1 z} \tag{20}$$

We examine three special cases:

- 1) $\alpha_1 = \beta_1 = 0$. In this case, $A^j = B^j = C^j = 0$. The simplest solution is $c_4 = 1$, $c_5 = c_6 = 0$.
- 2) $\beta_1 = 0$. In this case, $A^j = c^j = 0 \neq B^j$. Again the simplest solution is to set $c_4 = 1$, $c_5 = c_6 = 0$.
- 3) $\alpha_1 \neq 0 \neq \beta_1$. In this case we are free to choose $C_6 = 0$; then from (13), $A^j c_5 = C^j c_4$, and since the determinant is zero (A^{-2} , C^{-2}) equals (A^2 , C^2) within a constant factor so we can set $c_5 + C^2$ and $c_4 = A^2$. One could, of course, set c_5 and c_6 to any numbers not equal to 0; this would amount to multiplying numerator and denominator by the same factor, provided the overall polynominal remained of degree ≤ 2 .

Once the coefficients c_i have been obtained, the roots z_{n1} , z_{n2} , z_{d1} and z_{d2} are easily obtained. The integral is then performed from z_a to z_b where $z_a = \frac{z_{-1} + z_0}{2}$ and $z_b + \frac{z_0 + z_1}{2}$. If z_0 is not a corner point, that is, if $\Delta^2 z/\Delta z = 0$, then the integral is performed in one step: z_a to z_b : If $\Delta^2 z/\Delta z \neq 0$, it is performed in two steps, z_a to z_0 , and z_0 to z_b . The integrals are performed in the transformed coordinate system ($z_3 = 0$), the same one that the coefficients are found in.

III. DESCRIPTION OF THE SUBROUTINE

A. CAUCHY

The main subroutine begins by initializing IND (D = double precision), where N is defined in equation (1). The initialization is necessary, since the subroutine which performs the integral adds incrementally to IND.

Setting $C(1) = 10^{15}$ signals COEF that it is the first time that COEF has been called for a given contour (see description of COEF).

The array ZSC(I) is set equal to $|\Delta Z_i|$. If any ZSC(I) equals zero, an error message is printed out and a return initiated.

A check is made to see if the contour contains at least five points. If not, an error message is printed out and a return initiated.

The DO 160 loop is now started; this ultimately performs the incremental integral for each Z(I). Each set of five $z_j = ZD(J)$ and $f_j = FD(J)$, $1 \le J \le 5$ are then set up, with special provisions at the "beginning" and "ending" of the contour. For these five ZD(J) and FD(J), the coefficients $c_{\ell} = CD(L)$, $1 \le L \le 6$, are calculated (see equation (6)) in subroutine COEF. The roots ZRN(1) and ZRN(2) of the numerator, and ZRD(1) and ZRD(2) of the denominator, are calculated in ROOT2.

A check is then made to see if $\Delta^2 Z_3/\Delta Z_3 \simeq 0$; if so, the point ZD(3) is not a "corner point", and the integral is performed from [ZD(2)+ZD(3)]/2=Z1 to [ZD(3)+ZD(4)]/2=Z2. If ZD(3) is a corner point, the integral is done in two steps: from Zl to ZD(3), and from ZD(3) to Z2.

The integrals IN = IND, $0 \le N \le 2$ are divided by $2\pi i$ and then a return is made to the calling program.

B. COEF

Given the function F(I) at Z(I), $1 \le I \le 5$, this subroutine calculates the $c_j = C(J)$, $1 \le J \le 6$ as defined in (6).

A check is first made to see if $C(1) = 10^{15}$. If so, it is the first call of COEF for a given contour, and all five $|f_i| = FM(I)$, $1 \le I \le 5$ are calculated; if not, the FM(I) are set equal to the FM(I+1), $1 \le I \le 4$, and FM(5) is calculated from F(5).

From the FM(I), a scale factor is formed by finding the largest FM(I). If Max (FM(I)) = 0, F(I) = 0, $1 \le I \le 5$, and the scale factor is not needed; otherwise the scale factor SCF = $1/\max(FM(I))$.

All FM(J) are now multiplied by SCF. Then the second largest FM(I), TSCFM is found. If it is 0, then the largest F(I) = F(J) is a singular point, and the points of the contour have to be redefined. Hence an error message and stop are provided. If two or more FM(I) are equal to the maximum FM(I), or if the TSCFM \neq 0, the program proceeds. Note that the presence of two singular points at two contour points (within five consecutive points) would cause the program to fail without any error message.

The program now proceeds to calculate the A^{j} , B^{j} , C^{j} defined in equations (14), (15), and (16) ($A^{-2} \equiv AN2$, etc.). From these, C(4), C(5), and C(6) are calculated. We now test to see if C(4) = DET = 0. Since we have used the scaled FF(I) to calculate C(4), we define "0" as a small number to take care of roundoff errors in subtraction. If |C(4)| = "0", then we have a function of the type shown in equation (20).

We then set C(5) = C2 and C(4) = A2 as discussed in case 3). In addition |C(5)| = 0, we have either case 2) or case 1), and in either case, the denominator is a constant, set equal to 1. The numerator coefficient C(1), C(2), C(3) are then calculated, and the return is made to CAUCHY.

C. ROOT2

This program calculates the roots ZR(1) and ZR(2) of $f = A*Z^2 + B*Z + C$. Roots at infinity are set to 10^{27} . The subroutine then calculates $Z(1) = -B + \sqrt{B^2 - 4*A*C}$ and $Z(2) = -B - \sqrt{B^2 - 4*A*C}$. If $T_1 = |Z(1)| = 0$ and $T_2 = |Z(2)| = 0$ special cases must be treated. In that case, if A = 0, then f = constant, and the two roots are at "infinity"; a return is made. If C = 0 also (which could not happen in CAUCHY, but might arise in some other use of ROOT2), an error stop and message are instituted. If A = 0 when $T_1 = T_2^{20}$, then both roots ZR(1) = ZR(2) = 0.

If none of the special cases occurs, we determine the larger of T1 and T2. The larger Z(1,2) is then used to calculate ZR(1) = 2C/Z(1,2). A check is made to see whether the second root is at "infinity", corresponding to A = 0. If it is, a return occurs, if not the second root is calculated: ZR(2) + Z(1,2)/2A.

D. INCIN

Incin increments the I_O, I₁ and I₂ integrals by forming

$$I_{O} = I_{O} + FND \cdot \sum_{j=1}^{IR} \Delta I_{Oj}, \qquad (21.1)$$

$$I_1 = I_1 + FND \cdot \sum_{j=1}^{IR} \Delta I_{2j}$$
, (21.2)

and

$$I_2 = I_2 + FND \cdot \sum_{j=1}^{IR} \Delta I_{2j}$$
 (21.3)

where

$$\Delta I_{Oj} = \int_{Z1}^{Z2} \frac{dz}{(z - Z_j)}$$
 (22.1)

$$\Delta I_{1j} = \int_{Z1}^{Z2} \frac{z \, dz}{(z - Z_j)}$$
 (22.2)

and

$$\Delta I_{2j} = \int_{Z_1}^{Z_2} \frac{z^2 dz}{(z-Z_j)}$$
 (22.3)

Z1, Z2, FND, I ϕ , I1, I2 and IR are arguments of INCIN. The Z 's are obtained from

$$Z_{j} = ZC + ZR(J)$$
 (23)

where ZC and ZR(j) are additional arguments of the subroutine.

Starting with equations (22), ΔI_{lj} can be expressed as

$$\Delta I_{1j} = \int_{Z1}^{Z2} dz \frac{\left[(z-Z_j) + Z_j \right]}{(z-Z_j)}$$

$$= \int_{Z1}^{Z2} dz \left[1 + \frac{Z_j}{(z-Z_j)} \right]$$

$$= (Z2 - Z1) + Z_j \Delta I_{10}$$

$$= DZ + Z_j \Delta I_{10}$$

$$(24.1)$$

and

$$\Delta I_{2j} = \int_{Z_{1}}^{Z_{2}} dz \frac{\left[\left(z^{2} - Z_{J}^{2}\right) + Z_{j}^{2}\right]}{\left(z - Z_{j}\right)}$$

$$= \int_{Z_{1}}^{Z_{j}} dz \left[z + Z_{j} + \frac{Z_{j}^{2}}{z - Z_{j}}\right]$$

$$= \frac{1}{2} \left(z_{2}^{2} - Z_{1}^{2}\right) + Z_{j} \left(z_{2} - Z_{1}\right)$$

$$+ Z_{j}^{2} \Delta I_{0j}$$

$$= DZ \cdot Z_{B} + Z_{j} \cdot DZ + Z_{j}^{2} \Delta I_{0j}$$

$$= DZ \cdot Z_{B} + Z_{j} \cdot \Delta I_{1j}$$
(24.2)

where

$$DZ = Z_2 - Z_1$$
 (25.1)

and

$$Z_{B} = \frac{1}{2} (Z_{1} + Z_{2}).$$
 (25.2)

So the only difficulty is the evaluation of ΔI_{\cap} . If

$$z = \frac{1}{2} DZ \cdot x + Z_B$$

is substituted into equation (2.1) it is seen that

$$\Delta I_{Oj} = \int_{-1}^{1} \frac{dx}{x - \frac{2(Z_{j} - Z_{B})}{DZ}}$$
 (26)

or
$$\Delta I_{0j} = \int_{a}^{b} \frac{dx}{x - a - ib}$$
(27)

where

$$a + ib = \frac{2(Z_j - Z_B)}{DZ}$$
 (28)

and

a and b are real.

This can then be expressed as

$$\Delta I_{Oj} = \int_{-1}^{1} \frac{dx (x - a + i b)}{(x-a)^2 + b^2}$$

$$\frac{1}{2} \ln \left[(x-a)^2 + b^2 \right]_{-1}^{1} + ib \int_{-1}^{1} \frac{dx}{(x-a)^2 + b^2}$$
 (29)

$$= \frac{1}{2} \ln \left[\frac{(1-a)^2 + b^2}{(1+a)^2 + b^2} \right] + i b \int_{-1}^{1} \frac{dx}{(x-a)^2 + b^2} ,$$

and

Im
$$\Delta I_{0j} = b \int_{-1}^{1} \frac{dx}{(x-a)^2 + b^2}$$
 (30)

Now make the substitution

$$x = a + |b| \tan \varphi \tag{31}$$

with

$$\tan \varphi_{-1} = -\frac{(1+a)}{|b|},$$

$$\tan \varphi_1 = \frac{1-a}{|b|},$$

and

$$|\varphi| \le \frac{\pi}{2} \qquad , \tag{32}$$

into equation (30).

It is now seen that

$$\operatorname{Im} \Delta I_{O,j} = \frac{b}{|b|} \int_{\phi_{-1}}^{\phi_{1}} d\phi$$

$$= \frac{b}{|b|} (\phi_{1} - \phi_{-1}) . \tag{33}$$

Since -1 < 1 it follows from equation (31) and (32) that

$$0 \le \varphi_1 - \varphi_{-1} \le \pi$$

hence

$$|\operatorname{Im} \Delta I_{Oj}| \leq \pi$$
 (34)

Starting again with equation (26) it follows that

$$\Delta I_{Oj} = \int_{-1}^{1} \frac{dx}{x - \frac{2}{DZ} (Z_{j} - Z_{B})},$$

$$= \ln (x - \frac{2}{DZ} (Z_{j} - Z_{B}))^{1}_{-1},$$

$$= \ln \left(\frac{1 - \frac{2}{DZ} (A_{j} - Z_{B})}{-1 - \frac{2}{DZ} (Z_{j} - Z_{B})}\right),$$

$$= \ln \left(\frac{\frac{2}{DZ} (Z_{j} - Z_{B})}{-1 - \frac{2}{DZ} (Z_{j} - Z_{B})}\right),$$

$$= \ln \left(\frac{\frac{2}{DZ} (Z_{j} - Z_{B}) - 1}{\frac{2}{DZ} (Z_{j} - Z_{B}) + 1}\right),$$
(35)

with the branch specified by equation (34).

If

$$\left|\frac{2(Z_{j}^{-1}Z_{B})}{DZ}\right| \leq 1$$

define

$$R = \frac{2(Z_j - Z_B)}{DZ} \tag{36}$$

and then

$$\Delta I_{0,j} = \varrho_n \left(\frac{1-R}{1+R}\right) + \varrho_n (-1),$$

and

$$\Delta I_{0,j} = \varrho_n \left(\frac{1-R}{1+R}\right) - i\pi . \tag{37}$$

It makes no difference which branch of w(-1) is used here since the imaginary part of Δ I_{Oj} is adjusted to satisfy equation (34) by adding or subtracting 2π i to the final result.

If
$$1 \le \left| \frac{2 \left(Z_{j} - Z_{B} \right)}{DZ} \right|$$

then R is defined as

$$R = \frac{DZ}{2(Z_j - Z_B)}$$
 (38)

and

$$\Delta I_{Oj} = \ln \left(\frac{\frac{1}{R} - 1}{\frac{1}{R} + 1} \right)$$

$$= \ln \left(\frac{1 - R}{1 + R} \right)$$
(39)

This is the same as equation (37) without the - i π term.

The program sets R according to the value of $\left|\frac{(Z_j-Z_B)}{DZ}\right|$ to either the R.H.S. of equation (36) or (38) and Δ I_{Oj} to - i π or 0. Then in either case the fortran statement

$$\Delta I_{Oj} = \Delta I_{Oj} + CDLOG \left(\frac{1 - R}{1 + R}\right)$$

produces Δ I_{Oj}. If R is less than .1 an expansion of the ℓn $\left(\frac{1-R}{1+R}\right)$ is used otherwise a fortran supplied subrouting computes the value. The imaginary part of Δ I_{Oj} is adjusted to satisfy equation (34) by adding or subtracting 2 πi . Then Δ I_{Dj} and Δ I_{2j} are computed from equations (24) and the integrals are incremented.

IV. SAMPLE RESULTS

In Table 1, we show results for various functions when integrated around a square in the complex Z-plane

- 2
$$\leq$$
 Re, Im(Z) \leq 2

While the function does not provide an exhaustive examination, it does illustrate several important points

- 1) There is a dramatic change in the winding number (IO) as a zero or pole crosses a contour. In all examples, this zero or pole was chosen to lie halfway between two grid points by choosing an appropriate y.
- 2) The error in any two runs should decrease as $\left(\frac{\Delta Z}{\Delta Z} \frac{\text{Run B}}{\text{Run A}}\right)^{4}$; for the larger errors, this is borne out in practice.
- 3) Even a crude number of points, with zeros (or poles) right on the contour yield an interpretable IO.

In Table 1, the first column shows the function calculated. Results are listed for three different ΔZ . Below the calculated result is the correct result for comparison.

Table 1A

)-		\DZ = 1		
	f(z) `	IO .	Il	I2
	1 - z	1.0000+0.0000i 1+0i	1.0000+0.0000i 1+0i	1.000+0.000i 1+0i
	sin (z/4)	1.0001+0.0000i 1+0i	-0.0000+0.0000i 0+0i	-0.000+0.000i 0+0i
	$\frac{\sin (z/4)}{z-1}$	-0.0002-0.0000i 0+0i	-1.0003+0.0000i -1+0i	-1.005+0.000i -1+0i
	$\frac{\sin\left[\frac{z-1.99-iy}{4}\right]}{z-1}$	-0.0571+0.0048i 0+0i	0.8695+0.4814i .99+.5i	2.468+1.8 <i>9</i> 2i 2.710+1.99i
	$\frac{\sin\left[\frac{z-2.01-iy}{4}\right]}{z-1}$	-0.8860-c.0608i -1+0i	-0.7420-0.0659i -1+0i	-0.457-0.005i -1+0i
	$\frac{\sin\left[\frac{z-3}{4}\right]}{z-1}$	-1.0020+0.0000i -1+0i	-1.0026-0.0000i -1+0i	-1.004+0.000i -1+0i
	$\frac{\sin (z/4)}{z - 1.99 - iy}$	-0.0329+0.0041i 0+0i	-2.0586-0.5081i -1.995i	-3.850-2.041i -3.71-1.99i
	$\frac{\sin (z/4)}{z - 2.01 - iy}$	1.0332-0.0037i 1+0i	0.0675+0.0091i 0+0i	0.124+0.052i 0+0i
	$\frac{\sin (z/4)}{(z-1)(z+1)}$	-1.0009+0.0000i -1+0i	0.0000-0.0000i 0+0i	-1.985+0.000i -2+0i
	$\frac{\sin (z/4)}{(z-1)^2}$	-1.0002+0.0000i -1+0i	-1.9992+0.0000i -2+0i	-1.979-0.000i -2+0i

Table 1B

f(z)	IO	<u> </u> .5 I1	12
1 - z	1.000+0.000i	1.0000+0.0000i	1.000+0.000i
	l + 0i	1 + Oi	l + 0i
$\sin(z/4)$	1.0000+0.0000i	-0.0000+0.0000i	-0.0000+0.000
	l + 0i	0 + Oi	0 + Oi
$\frac{\sin(z/4)}{-1}$	-0.0000+0.000i	-1.0000+0.0000i	-1.000+0.000i
_	0 + Oi	-1 + Oi	-1 + Oi
$\frac{\sin\left[\frac{z-1.99-iy}{4}\right]}{z-1}$			
z - 1	-00052+0.0010i	0.9793+0.2508i	2.875 + 0.994i
Fr 0 01 :	0 + 0i	.99 + .25i	2.898 + 0.995i
$\frac{\sin\left[\frac{z-2.01-iy}{4}\right]}{z-3}$	-0.9941-0.0012i	0.0878 0.0033	0.07(
z - 1	-1 + 0i	-0.9878-0.0011i -1 + 0i	
[, 3,]	1 01	-1 + 01	-1 + Oi
$\frac{\sin\left[\frac{z-3}{4}\right]}{z-3}$	-1.001+0.0000i	-1.0002-0.0000i	1 000 0 000
z = 1	-1 + Oi	-1 + 0i	-1.000-0.000 -1 + 0i
		2 01	-1 · OI
$\frac{\sin(z/4)}{z-1.99-iv}$	-0.0011+0.003i	-1.9923-0.2498i	-3.903-0995i
z -1 . 99-1 y	0 + 0i	-1. 99 - 0.25i	-3.898-0.995i
			J. 0, 0 = 0 • 7, 7, 7 ±
$\frac{\sin(z/4)}{z-2.01-iy}$	1.0012-0.0003i	0.0025-0.0003i	0.005+0.000i
	1 + Oi	0 + Oi	0 + Oi
sin(z/4)		• •	
$\frac{\sin(z/4)}{(z-1)(z+1)}$	-1.0002-0.0000i	0.0000-0.0000i	-1.999-0.000i
	- 1 + Oi	0 + Oi	- 2 + 0
sin(z/4)	-1.0001+0.0000i	2 0002 0 00003	1 009 0 000
$\frac{\sin(z/4)}{(z-1)^2}$	-1.0001+0.00001 - 1 + 0i	-2.0001-0.0000i -2 + 0i	-1.998-0.000i
	- T - OI	- 2 + U1	- 2 +0i

Table 1C

	Δz .25				
f(z)	IO	Il	I2		
1 - z	1 + Oi	l + 0i	l + Oi		
	1 + Oi	1 + Oi	1 + Oi		
sin(z/4)	1 + Oi	0 + Oi	0 + Oi		
	1 + Oi	0 + Oi	0 + Oi		
$\frac{\sin(z/4)}{z-1}$	0 + Oi	-1 + Oi	-1 + Oi		
2 - 1	0 + Oi	-1 + Oi	-1 + Oi		
$\sin\left[\frac{z-1.99-iy}{4}\right]$	-0.0003+0.000li	0.9894+0.1251i	5 0/12+0 1/08+		
z - 1	0 + Oi	·99 + ·125i			
$\frac{\sin\left[\frac{z-2.01-iy}{4}\right]}{z-1}$ $\sin\left[\frac{z-3}{4}\right]$	0.9996-0.000li -1 + 0i -1 + 0i	-0.9993-0.000li -1 + 0i	-1 + Oi		
$\frac{\sin\left[\frac{z-3}{4}\right]}{z-1}$	-1 + Oi	-1 + 0i -1 + 0i	-1 + Oi -1 + Oi		
sin(z/4) z-1.99-iy	0.0000+0.0000i 0 + 0i	-1.99901-0.1250i 1.99-0.25i	-3.945-0.498i -3.944-0.498		
sin(z/4) z-2.01-iv	1 + Oi	0 + 0i	0 + 0i		
z-2.01-iy	1 + Oi	Q + Oi	0 + Oi		
sin(z/4) z-1)(z+1)	1 + Oi 1 + Oi	0 + 0i 0 + 0i	0 + 0i		
	<u> </u>	0 , 01	0 + Oi		
$\frac{\sin(z/4)}{(z-1)^2}$	-1 + Oi	-2 + Oi	-2 + Oi		
(z-1) ^{<}	-1 + Oi	- 2 + 0i	-2 + 0i		

REFERENCES

- 1. J. E. McCune, Phys. Fluids <u>9</u>, 2082 (1966).
- 2. Applications Program Series AP-26, Mass. Inst. of Tech. Information Processing Center, March 28, 1973.

```
C
      SUBROUTINE CAUCHY (IMAX, Z, F, 10, 11, 12)
C
      CAUCHY CALCULATES THE INTEGRALS IS=INT(D(LN(F))/DZ)/2+PI+I,
C
     11 = INT (Z+D(LN(F))/DZ)/2+PI+I, AND IZ=INT (Z++2+D(LN(F))/DZ)02+PI+I
C
Č
      WHERE F IS DEFINED AT IMAX POINTS ON THE CONTOUR Z. IN COEF
      THE CURVE IS FIRST FIT TO A FORM (ARX##2+BRX+C)/(DRX##2+E#X+F),
C
Ç
      THE ROOTS OF THE NUMERATOR AND DENOMINATOR ARE OBTAINED (ROOTZ),
      AND THEN THE INTEGRAL IS PERFORMED (INCIN)
C
      COMPLEX*16 ZD(5),FD(5),CD(6),ZRN(2),ZRD(2),Z1,Z2,IØD,I1D,I2D
      COMPLEX#8 I(101), F(101), I0, I1, I2
      REAL#4 Z8C(101)
C
      100 = (0.00,0.00)
      110=(0.00,0.00)
      120 = (0.00,0.00)
      CD(1) = (1.015,0.00)
      DO 110 I=2, IMAX
      Z8C(I) = CABB(Z(I) = Z(I=1))
      IF(Z8C(I).NE.0.) GO TO 110
      WRITE (1,501)
  501 FORMAT (19H ERROR IN Z-CONTOUR)
      RETURN
  118 CONTINUE
      IF (IMAX.GE.5) GO TO 120
      WRITE (1,502)
 502 FORMAT (10H IMAX.LT.5)
      RETURN
 120 IMAXM1=IMAX=1
      DO 168 I=1, IMAXM1
      DO 130 J=1,5
      L+E-I=LL
      IF(JJ.EQ.-1) JJ=IMAX-2
      IF(JJ.EG.Ø) JJ=IMAX-1
      IF(JJ.GT.IMAX) JJ=2
      ZD(J) = Z(JJ)
 130 FD(J) = F(JJ)
      CALL COEF(ZD,FD,CD)
      CALL ROOT2(CD(1),CD(2),CD(3),ZRN)
      CALL ROOT2(CD(4),CD(5),CD(6),ZRD)
      IP=I+1
      IMPI-1
      IF(IM.EQ.O) IM=IMAX=1
      IF(CABS(Z(IP)+Z(IM)+2.+Z(I)).LT.ZSC(IP)+1.E+6) GO TO 140
      Z1#(Z(I)+Z(IM))*0.5
      Z2#Z(I)
     CALL INCIN(Z1, Z2, ZD(3), ZRN, 2, 10D, 11D, 12D, 1.D0)
     CALL INCIN(Z1, Z2, ZD(3), ZRD, 2, IØD, I1D, I2D, -1, DØ)
      Z1=Z(I)
     22=(Z(IP)+Z(I))+0.5
     GO TO 150
 140 \ Z1 = (Z(I) + Z(IM)) *0.5
     Z2=(Z(IP)+Z(I))*0.5
 150 CALL INCIN(Z1, Z2, ZD(3), ZRN, 2, I0D, I1D, I2D, 1.D0)
     CALL INCIN(Z1, Z2, ZD(3), ZRO, 2, I@D, I1D, I2D, -1.D@)
 168 CONTINUE
     10:100/(0.00,6,283185300)
     I1=I1D/(0.D0,6.2831853D0)
     12=120/(0.00,6.2831853D0)
     RETURN
     END
                                         21
```

```
SUBROUTINE INCIN(Z1,Z2,ZC,ZR,IR,I0,I1,I2,FND)
      IMPLICIT COMPLEX+16 (A-H, O-Z)
      INCIN ADDS THE INCREMENTAL INTEGRALS FROM Z1 TO Z2 TO THE
C
      INTEGRALS ID. II. AND IZ.
      I-SUB-N # I-SUB-N + FND * SUM OVER J, J=1, IR OF INT(J), WHERE
Ĉ
      INT(J) = INTEGRAL FROM Z1 TO Z2 OF (DZ+(Z++N)/(Z-ZC-ZR(J))
C
      REAL+& AR, PI, TWOPI, FND, TEST
      COMPLEX+16 10, 11, 12, ZR(1)
      DATA PI/3.1415926535897900/, TWOPI/6.2831853071795800/
      DZ=Z2-Z1
      Z8=.500+(Z2+Z1)
      00 50 J=1, IR
      ZJ=ZR(J)+ZC
      ZRB=2.00*(ZJ-ZB)
      R=ZRB/DZ
      AR#CDABS(R)
      IF(AR.GT.1.00) GO TO 10
      DISDCMPLX(@.DO. -PI)
      GO TO 20
      R=DZ/ZRB
10
      AR=1.DØ/AR
      DI=(0.00,0.00)
20
      IF(AR.GT.0.100) GO TO 30
      IF(AR.LT.1.0=25) GO TO 50
     RSBRWR
     DI#DI=R*(2.00+(.66666666666666700+(.400+(.285714285714285700
    1 +(.2222222222222200+.1818181818181818D0*RS)*RS)*RS)*RS)*RS)
     TEST DIMAG(DI)
     IF(TEST.LT.=PI) DI=DI+DCMPLX(0.D0,TWOPI)
     GO TO 40
30
     DI=DI+COLOG((1.00-R)/(1.00+R))
     TEST=DIMAG(DI)
     IF(TEST.GT.PI) DI=DI=DCMPLX(0.D0,TWOPI)
     IF(TEST.LT.-PI) DI=DI+DCMPLX(0.D0,TWOPI)
40
     IO=IO+FND+DI
     DI=DZ+ZJ*DI
     I1=I1+FND+DI
     I2=I2+FNO+(DZ+ZB+ZJ+DI)
50
     CONTINUE
     RETURN
     END
```

```
SUBROUTINE ROOT2(C, 5, A, ZR)
      FINDS ROOTS OF A#Z##2+8#Z+C
CCC
      COMPLEX+16 A,B,C,ZR(2),Z(2),RAD
      REAL #4 T1, T2, TOVFL
C
      INFINITY = 1.027
C
      ZR(1)=(1.D27,0.D0)
      ZR(2) # (1.D27,0.D0)
      RAD=CDSQRT(B+B-4+A+C)
      Z(1)==B+RAD
      Z(2) ==B=RAD
       TI=CDABS(Z(1))
       T2=CDAB8(2(2))
       IF (T1+T2.NE.0.) GO TO 30
       IF(CDAB8(A).NE.0.) GO TO 20
       IF (CDABS (C) . NE. 0.) GO TO 10
      WRITE (51,501)
  501 FORMAT (* ERROR STOP
       STOP
   10 RETURN
   28 ZR(1)=(0,00,0.00)
       ZR(2) = (0.00,0.00)
       RETURN
   30 I+1
       IF(T2.GT.T1) I=2
       ZR(1)=(C+C)/Z(I)
       TOYFL#CDABS(1.D-27+Z(I))-CDABS(A+A)
       IF(TOVFL.GT.Ø.) RETURN
       ZR(2)=Z(I)/(A+A)
       RETURN
       END
```

```
SUBROUTINE COEF(Z,F,C)
C
C
       PROGRAM TO FIND COEFFICIENTS FOR THE FUNCTION
       F=(C(1)+C(2)+Z+C(3)+Z**2)/(C(4)+C(5)+Z+C(6)+Z**2)
C
Č
       GIVEN THE FUNCTION F AT FIVE POINTS Z.
C
       IMPLICIT COMPLEX#16 (A=H,O=Z)
       DIMENSION Z(5), F(5), C(6), FF(5)
      REAL+8 ZERO/1.D-10/, SCF, FM(5), TSCF(5), TSCFM
C
Č
      DETERMINE SCALE FACTOR (SCF) FOR F SO F IS OF ORDER ONE
C
      IF(CDAB8(C(1)).NE.CDAB8((1.D15,0.D0))) GO TO 20
      DO 10 I+1.5
   10 FM(I) #CDABS(F(I))
      60 TO 46
   20 DO 30 1=1.4
   30 FM(I) = FM(I+1)
      FM(5) = CDABS(F(5))
   40 SCF=DMAX1(FM(1),FM(2),FM(3),FM(4),FM(5))
      IF (SCF.NE.0.D0) SCF=1.D0/SCF
C
      DETERMINE IF FUNCTION IS SINGULAR (TSCFM=0).
C
                                                       IF ITSCF.GT.1.
C
      FUNCTION IS CONSTANT AT TWO OR MORE POINTS.
      ITSCF=0
      DO 50 I=1,5
      TSCF(I)=SCF+FM(I)
      IF (DABS (TSCF (I) -1.DU) .GT.ZERO) GO TO 50
      ITSCF#ITSCF+1
      J=I
   50 CONTINUE
      IF (ITSCF.GE.2) GO TO 70
      TSCFM=0.D0
      DO 60 I=1.5
      IF(1.EQ.J) GO TO 60
      IF (TSCF(I).GT.TSCFM) TSCFM=TSCF(I)
   68 CONTINUE
      IF (TSCFM.GT.ZERO) GO TO 70
      WRITE (51,501) (F(1),1=1,5)
  501 FORMAT (" ERROR STOP - SINGULAR FUNCTION: ", /1P10E12.4)
      STOP
   70 DO 80 I=1.5
   80 FF(I)=SCF+F(I)
C
      ZN2=Z(1)-Z(3)
      ZN1=Z(2)=Z(3)
      21=2(4)-2(3)
      Z2=Z(5)=Z(3)
C
      GN2=(FF(1)=FF(3))/ZN2
      GN1=(FF(2)-FF(3))/ZN1
      G1 = (FF(4) - FF(3))/21
      G2=(FF(5)-FF(3))/Z2
```

```
ZOENOM#1.00/(Z1-ZN1)
   F1M1=FF(4)=FF(2)
   ZF1=Z1+FF(4)
   ZF1M1#ZF1#ZN1*FF(2)
   G1M1=G1+GN1
   RAT = (ZN2=Z1) + ZDENOM
   AN2#RAT#F1M1#FF(1)#FF(4)
   BN2=RAT+ZF1M1=ZN2+FF(1)+ZF1
   CN2=GN2-G1-RAT+G1M1
   RAT= (Z2-Z1) +ZDENOM
   A2=RAT+F1M1+FF(5)+FF(4)
   B2#RAT#ZF1M1#Z2#FF(5)+ZF1
   C2=G2-G1-RAT+G1M1
   C(4) #A2+BN2-AN2+B2
   C(5) = C2 + BN2 + CN2 + B2
   C(6) = A2 + CN2 = AN2 + C2
   TEST FOR CASES WHERE DENOMINATOR COEFFICIENTS VANISH.
   IF(CDABS(C(4)),GT,ZERO) GO TO 90
   C(4) =A2
   C(5) =C2
   C(6) = (0.00, 0.00)
   IF(CDABS(C(5)).LE.ZERO) C(4)+(1.D0,0.D0)
90 C(3) = ZDENOM+ (G1M1+C(4)+F1M1+C(5)+ZF1M1+C(6))
   C(2) == Z1 *C(3) +G1 *C(4) +FF(4) *(C(5) +Z1 *C(6))
   C(1) #FF(3) #C(4)
   RETURN
   END
```

C

C

C