

## Programs and Listings

### Introduction

It is the intention in this Addenda to provide the reader of my book “Numerical Methods for Laplace Transform Inversion” with a variety of programs to evaluate the inverse Laplace transform. The only requirement is the ability to write simple Fortran routines to evaluate the transform function  $\bar{f}(s)$ . As a general rule the programs require the use of double precision arithmetic - this is particularly the case with NAG library routines - but because the extrapolation methods used involve a lot of cancellation it is preferable to work with multi-precision arithmetic. It has been the policy of the author to indicate double/multiple precision variables by using the term **real**, that is real in bold characters, and also to indicate constants of this form by writing them in bold type. Thus **0.01** would represent 1d-2 in double precision or 1q-2 in quadruple precision and **10<sup>-10</sup>** would represent 1d-10 or 1q-10. Similarly, **complex** represents double/multiple precision complex variables. Likewise **exp** represents dexp in double precision and qexp in quadruple precision and indicates that the exponential operation will produce numerical results which are compatible with the variable declaration. Similarly for **sin**, **cos**, **abs**, **float**, and so on. For some functions we have used the generic name in the program. Examples of this are max, min and ifix where, depending on the computer used and the context we might require dmax1, dmin1 or jifix respectively — or some similar function names.

We now give examples of various programs and their specifications. It should be borne in mind that the parameters needed to operate some programs need careful choosing and it would be advisable to rerun the programs with alternative parameter settings. While the author has attempted to write optimal programs for routines which have not been published this objective might not have been achieved in all cases. Additionally, the user has to be aware of the fact, especially when supplying  $\bar{f}(s)$  which is to be evaluated for complex values of  $s$ , of the need to determine the principal value of  $\bar{f}(s)$ .

Also included in this Chapter are two Mathematica programs. Some additional Mathematica programs can be found from the package LaplaceAndzTransforms — see Graf [5]. Further details relating to the NAG programs can be found at their website [9].

### Program for Weeks's method

This is based on the paper by Garbow et al [4] which determines a Laguerre series approximation  $\tilde{f}(t)$  to  $f(t)$  of the form

$$\tilde{f}(t) = e^{\sigma t} \sum_{i=0}^{m-1} a_i e^{bt/2} L_i(bt), \quad \sigma > \sigma_0, \quad b > 0$$

where  $\sigma_0$  ( $=\gamma$ ) is the abscissa of the singularity of  $\bar{f}(s)$  which is furthest from  $\Re s = 0$ . NAG routine C06LBF computes the coefficients  $a_i$  and the routine C06LCF evaluates the expansion for specified  $t$ .

### Entry/Exit Parameters

1.  $f$  — **complex** function to be supplied by user.  $f$  must return the value of the Laplace transform  $\bar{f}(s)$  for given  $s$ .
2.  $\text{sigmao}$  — **real**. The value of  $\sigma_0$ .
3.  $\text{sigma}$  — **real**, the parameter  $\sigma$  of the Laguerre expansion. It is replaced by  $\sigma_0 + 0.7$  on exit if  $\sigma < \sigma_0$ .
4.  $b$  — **real**. If  $b < 2(\sigma - \sigma_0)$  on entry it is replaced by  $2.5(\sigma - \sigma_0)$ .
5.  $\text{epstol}$  — **real**. An upper bound on  $|f(t) - \tilde{f}(t)|e^{-\sigma t}$ .
6.  $\text{nmax}$  — integer. An upper bound for the number of coefficients actually computed. It is recommended that  $\text{nmax}$  is a power of 2 ( $\geq 8$ ) and 1024 is sufficient in most cases.
7.  $m$  — integer. The number of Laguerre expansion coefficients actually computed.
8.  $\text{acoef}(\text{nmax})$  — **real** array. On exit, the first  $m$  elements contain the computed coefficients  $a_i$ .
9.  $\text{errvec}(8)$  — **real** array. On exit contains diagnostic information. In particular,  $\text{errvec}(1)$  contains an overall estimate for  $|f(t) - \tilde{f}(t)|e^{-\sigma t}$ . The NAG Library Manual should be consulted for further information.
10.  $\text{ifail}$  — integer. On exit  $\text{ifail}=0$  unless the routine detects an error. The NAG Library Manual should be consulted for details about the setting of  $\text{ifail}$  on entry and the significance of the output values of  $\text{ifail}$ .
11.  $t$  — **real**. On entry is the value of  $t$  for which  $f(t)$  is required.
12.  $\text{finv}$  — **real**. On exit the approximation of the inverse Laplace transform at  $t$ .

Full details of the application of the routines can be found in the NAG Library Manual. There follows a sample program to determine the inverse Laplace transform at the values  $t_i$ ,  $i = 1, \dots, n$  which

are to be read into the computer.

```
c      This is an application of NAG Library Routines C06LBF/C06LCF
integer nmax, nout
parameter(nmax=512, nout=6)
real b, epstol, exact, finv, pserr, sigma, sigmao, t
integer ifail, j, m
real acoef(nmax), errvec(8)
external C06LBF, C06LCF
complex f
external f

sigmao = 0.1
epstol = 0.00001
ifail=0
call C06LBF(f, sigmao, sigma, b, epstol, nmax, m, acoef, errvec, ifail)
write(nout,999) 'number of coefficients=', m
write (nout,*) '      t      f(t)      '

read(5,*)n
c      reads number of values of  $t$  at which  $f(t)$  required
do i=1,n
read(5,*)t
call C06LCF(t, sigma, b, m, acoef, errvec, finv, ifail)
write(nout,998)t,finv
enddo
stop
999  format(1x, a, i6)
998  format(1x, 1p, d10.2, d15.4)
end

complex function f(s)
c       $\bar{f}(s)$  is the transform of  $J_0(t)$ 
complex s, z
real pr, pi, qr, qi
external A02AAF
c      The NAG routine A02AAF evaluates complex square roots
z=s*s+1
pr=real(z)
```

```
pi=imag(z)
call A02AAF(pr, pi, qr, qi)
z=complex(qr, qi)
f= (1.0)/z
return
end
```

## Padé Table Construction by method of Longman

The program LONGPAD

Given a series

$$g(s) = a_0 + a_1s + a_2s^2 + \cdots + a_ns^n + \cdots$$

the program LONGPAD determines the Padé approximants

$$\frac{\beta_0 + \beta_1s + \cdots + \beta_ps^p}{\gamma_0 + \gamma_1s + \cdots + \gamma_qs^q},$$

for  $0 \leq p, q \leq [(n-1)/2]$ .

### Entry/Exit Parameters

1.  $n$  — integer. This should be an odd number and declared as a parameter.
2.  $a(i)$  — **real**. These are the coefficients in the series which have to be provided by the user.
3.  $b(i, j, k)$  — **real** array. On exit will correspond to the  $\beta_k$  of the  $[i/j]$  Padé approximant.
4.  $g(i, j, k)$  — **real** array. On exit will correspond to the  $\gamma_k$  of the  $[i/j]$  Padé approximant — see Longman [7]

The program below computes the diagonal terms in the Padé table for the function  $s\bar{f}(s)$  of Chapter 6, §3.

```
c      Requires the coefficients  $a_i$  in the Taylor series expansion
      parameter (n=11)
      real a(0:n), g(0:n, 0:n, 0:n), b(0:n, 0:n, 0:n), sig
      read(5,*)sig
      a(0)=1.0
      a(1)=-1.0
      a(2)=(1+sig)/2
      sig=sig/2
      do i=3, n-1
      call coeff(i,sig,a)
      write(6,*)i, a(i)
      enddo
      call longpad(n, a, b, g)
      m=(n-1)/2
```

```

do k=0, m
write(6,*)g(m, m, k), b(m, m, k)
enddo
stop
end

subroutine longpad(n, a, b, g)
real a(0:n), g(0:n, 0:n, 0:n), b(0:n, 0:n, 0:n), x, c(0:n)
if (n.le.25) goto 100
write(6,*)'n too large (> 25)'
stop
100 c(0)=1.0
c(1)=-a(1)/a(0)
do i=2, n-1
x=a(i)
do j=1, i-1
x=x+c(j)*a(i-j)
enddo
c(i)=-x/a(0)
write(6,*)i, c(i)
enddo

do j=0, n-1
do k=0, j
g(j, 0, k)=c(k)
b(0, j, k)=a(k)
enddo
enddo

do i=1, n-1
m=n-i
do j=0, m
b(i, j,0)=a(0)
enddo
enddo

do j=1, n-1
m=n-j
do i=0, m

```

```

g(i, j, 0)=1.0
enddo
enddo

do i=1, n-2
m=n-i
do j=1, m
do k=1, j
x=b(i-1, j, k-1)*b(i-1, j+1, j+1)/b(i-1, j, j)
b(i, j, k)=b(i-1, j+1, k)-x
enddo
enddo
enddo

do j=1, n-2
m=n-j
do i=1, m
do k=1, i
x=g(i, j-1, k-1)*g(i+1, j-1, i+1)/g(i, j-1, i)
g(i, j, k)=g(i+1, j-1, k)-x
enddo
enddo
enddo
return
end

subroutine fact(k, fac)
real fac
fac=1.0
if (k.eq.0) goto 100
do j=1, k
fac=j*fac
enddo
100 return
end

subroutine coeff(k, sig, a)
real c(k), a(k), y, sig
y=1.0

```

```

call fact(k, fac)
c(0)=y/fac
call fact(k-2, fac)
c(1)=y/fac
if (k.gt.3) goto 100
c(2)=(3*y)/2
goto 200

100  do i=2, k-1
      c(i)=y
      do j=k-i+2, k+i-2, 2
        c(i)=j*c(i)
      enddo
      call fact(k-i-1, fac)
      c(i)=c(i)/fac
      call fact(i, fac)
      c(i)=c(i)/fac
    enddo

200  a(k)=c(k-1)
      do i=k-2, 0, -1
        a(k)=a(k)*sig+c(i)
      enddo
      do i=1, k
        a(k)=-1.0*a(k)
      enddo
      return
end

```

### Program for Sidi's method of Laplace Inversion

This program is based on the variation of Sidi's method given in §5.3 . The user has to supply two function subroutines fun1(c,x,t,f) and fun2(c,x,t,f). The former will work out  $\Re \bar{f}(s)$  for given t and place it in location f, where  $s = c + it$ . The latter likewise works out  $\Im \bar{f}(s)$ . Numerical integration is performed by means of a Gauss 64-point quadrature formula for  $\int_0^1 g(x)dx = \sum_1^{64} w_i g(x_i)$ . For smaller t it might be preferable to use a higher order Gaussian quadrature formula or an adaptive approach based on the 64-point formula.

#### Entry/Exit Parameters.

1. t — a **real** number corresponding to the value at which the inverse transform is required.
2. c — a **real** parameter which has been set at **0.2** but must be increased to ensure that c is greater than the real part of any singularity of  $\bar{f}(s)$ .
3. x — a **real** variable which equals  $\Im s$ . This is required for the function subroutines fun1 and fun2.
4. n — integer, the number of points used by the Gauss quadrature rule. The default value is 64. A change in n would require an update of the subroutine gauss(n,x,w).
5. m — integer, the number of terms used in the mW - extrapolation. The default value is 40 but this can be altered as long as it is not too drastically different.
6. a — **real**, on exit should be a good approximation to the inverse transform if it agrees with b.
7. b — **real**, on exit should be a good approximation to the inverse transform if it agrees with a.

If a and b are not equal then the calculation should be repeated with the "c" qualifying the print instruction suppressed in the subroutine extrap. If the successive iterations show some consistency for a, say, then a can be accepted as an approximation to the transform. (See Chapter 10).

```
parameter (n=64, m=40)
real x(n), w(n), a, b, t, c, pi, xa, xb, ga, gb
real psia(0:m), fa(0:m),za(0:m+1)
real psib(0:m), fb(0:m), zb(0:m+1)
parameter (c=0.2)
```

```

write(6,*)'n=', n, 'm=', m, 'c=', c
pi=acos(-1.0)
read(5,*)t
do i=1, m+1
za(i-1)=(i*pi)/t
zb(i-1)=za(i-1)
enddo
za(0)=za(0)/2
call gauss(n, x, w)

fa(0)=0
k=0
psia(k)=0
do i=1, n
xa=k*za(0)+za(0)*x(i)
call fun1(c, xa, t, ga)
psia(k)=psia(k)+w(i)*ga
enddo
psia(k)=(pi*psia(k))/2

fb(0)=0
psib(k)=0
do i=1, n
xb=k*zb(0)+zb(0)*x(i)
call fun2(c, xb, t, gb)
psib(k)=psib(k)+w(i)*gb
enddo
psib(k)=pi*psib(k)
c write(6,*)k, psia(k), psib(k)

do k=1, m
psia(k)=0
psib(k)=0
do i=1, n
xa=(2*k-1)*za(0)+2*za(0)*x(i)
xb=k*zb(0)+zb(0)*x(i)
call fun1(c, xa, t, ga)
psia(k)=psia(k)+w(i)*ga
call fun2(c, xb, t, gb)

```

```

psib(k)=psib(k)+w(i)*gb
enddo
psia(k)=psia(k)*pi
fa(k)=fa(k-1)+psia(k-1)
psib(k)=psib(k)*pi
fb(k)=fb(k-1)+psib(k-1)
c write(6,*)fa(k), fb(k)
enddo

call extrap(m, psia, fa, za, a)
a=2*a/pi
a=(a*exp(c*t))/t
write(6,*)'a=', a
call extrap(m, psib, fb, zb, b)
b=2*b/pi
b=(b*exp(c*t))/t
write(6,*)'b=', b
stop
end

subroutine fun1(c, x, t, f)
c This subroutine evaluates  $\Re e^{-4\sqrt{s}}$ 
real c, x, t, f, u, v
complex s, w
s=complex(c, x)
w=-4.0*sqrt(s)
c sqrt denotes complex square root
w= exp(w)
f= real(w)
f=f* cos(t*x)
return
end

subroutine fun2(c, x, t, f)
c This subroutine evaluates  $\Im e^{-4\sqrt{s}}$ 
real c, x, t, f, u, v
complex s, w
s=complex(c, x)
w=-4.0*sqrt(s)

```

```

c      sqrt denotes complex square root
      w= exp(w)
      f= imag(w)
      f=-f* sin(t*x)
      return
      end

      subroutine extrap(m, psi, f, z, a)
      real psi(0:m), f(0:m), z(0:m), p(0:m), q(0:m), a, b
      do j=0, m
      p(j)=f(j)/psi(j)
      q(j)= 1.0/psi(j)
      enddo
      do k=1, m
      do j=0, m-k
      p(j)=p(j+1)-p(j)
      q(j)=q(j+1)-q(j)
      b=( 1.0/z(j+k))-(1.0/z(j))
      p(j)=p(j)/b
      q(j)=q(j)/b
      enddo
      a=p(0)/q(0)
c      write(6,*)a
c      the write statement in previous line should be reinstated
c      if there is a significant difference between the
c      estimates 'a' and 'b' for the Laplace transform
      enddo
      return
      end

      subroutine gauss(n, x, w)
      real x(n), w(n)
      x(1)=0.999652520867886069728452812172818
      w(1)=0.0008916403608482164736480395724898344
      x(2)=0.998170058385977639673462250338200
      w(2)=0.002073516630281233817643767864276530
      x(3)=0.995506685738372160369691191721652
      w(3)=0.003252228984489181428058680199989531
      x(4)=0.991668126942312958465649651078416

```

w(4)=0.004423379913181973861515457329864311  
x(5)=0.986663413894955481870926753676136  
w(5)=0.005584069730065564409295246509604289  
x(6)=0.980504399826026859459307060948579  
w(6)=0.006731523948359321299030383342978218  
x(7)=0.973205687429201408031240745673632  
w(7)=0.007863015238012359660982997648769673  
x(8)=0.964784586065969787910745077279613  
w(8)=0.008975857887848671542522651000559224  
x(9)=0.955261068539251402878190334004165  
w(9)=0.01006741157676510468617015836427180  
x(10)=0.944657722997557052926702019136426  
w(10)=0.01113508690419162707964916519207727  
x(11)=0.932999699077046409880391692535079  
w(11)=0.01217635128435543666908877520453430  
x(12)=0.920314648126290181375845772347937  
w(12)=0.01318873485752732933584589631261280  
x(13)=0.906632657561398779870961669043152  
w(13)=0.01416983630712974161375565260011866  
x(14)=0.891986179471670703805110262606884  
w(14)=0.01511732853620123943398702990977421  
x(15)=0.876409953630265948305931887442847  
w(15)=0.01602896417742577679273375217394922  
x(16)=0.859940925085805413424470108915974  
w(16)=0.01690258091857080469578274105536263  
x(17)=0.842618156527116621281779185515688  
w(17)=0.01773610662844119190534657335762311  
x(18)=0.824482735627328669928880615996702  
w(18)=0.01852756427012002302020755090479165  
x(19)=0.805577677586196625124426485509274  
w(19)=0.01927507658930781456448124847340455  
x(20)=0.785947823101317017141939058329594  
w(20)=0.01997687056636017069332846306416800  
x(21)=0.765639732009947272829006951772228  
w(21)=0.02063128162131176430507814873681898  
x(22)=0.744701572853526478739263153510961  
w(22)=0.02123675756182679450366988395440869  
x(23)=0.723183008626732043992473857379458  
w(23)=0.02179186226466172668841393048686875

```

x(24)=0.701135078981995801847883385630079
w(24)=0.02229527908187828153006735501547241
x(25)=0.678610079168834057975221307523101
w(25)=0.02274581396370907223988549848563456
x(26)=0.655661435995105478078756349280078
w(26)=0.02314239829065720864797662461613062
x(27)=0.632343581104383708186982086255010
w(27)=0.02348409140810500866266314287729056
x(28)=0.608711821870003542074824374494411
w(28)=0.02377008285741515433114110347211160
x(29)=0.584822210211996409018656814874135
w(29)=0.02399969429822915386406308993567301
x(30)=0.560731409648060277235188231746124
w(30)=0.02417238111740147858488476357900890
x(31)=0.536496560893899519724771470970169
w(31)=0.02428773372075171346739953339198905
x(32)=0.512175146331712216254477921426858
w(32)=0.02434547850456986019168269536737497
j=n/2
do i=1, j
x(j+i)=1-x(j-i+1)
w(j+i)=w(j-i+1)
enddo
return
end

```

**Implementation of the  $d^{(m)}$ -transformation via the  $W^{(m)}$ -Algorithm**

The  $W^{(m)}$ -Algorithm is a way of implementing the  $d^{(m)}$  transformation — see §12.4, Ford and Sidi [3] and Sidi [10].

**Entry/Exit Parameters.**

1. `cf(I)` — **real** array which contain the elements of the series to be summed. In the program which follows the program is applied to two cases of series summation where the general terms are respectively  $(1/n^{3/2} + 2/n^2)$  and  $(\cos n)/n$  and also to finding the limit of the Post-Widder sequences relating to  $\bar{f}(s) = 1/(s+1)$  and  $\bar{f}(s) = 1/\sqrt{(s^2+1)}$  (see §8.1).
2. `m` — integer. `m` specifies the transformation being used and must lie between 1 and `mdim` (`mdim` is usually chosen to be 6). For the two series considered one should take `m=2` and we can take `m=1` for the Post-Widder applications.
3. `lmax` — integer which specifies the number of terms of the series to be computed and which must be less than `ldim`.
4. `kappa` — **real**. This must be  $\geq 1.0$  and is required for arithmetic progression sampling (`aps`).
5. `sigma` — **real**. This must be  $\geq 1.0$  and is required for geometric progression sampling. `sigma` must be 1 for `aps` to be invoked
6. `epsdiv` — **real**. A small number which is used in testing the magnitude of the approximation `approx(j,p)`.
7. `approx(j,p)` — **real** array with  $0 \leq j \leq \text{ldim}$ ,  $0 \leq p \leq \text{ldim}$ . These approximations are returned by the  $d^{(m)}$  transformation
8. `cf(I)` — a function subprogram which has to be supplied by the user. In the case of the Post-Widder applications the value of `t` required in the Laplace inversion must also be supplied.
9. `np` — integer giving the specific sequence whose limit is required.

```
c      Implementation of the Ford-Sidi  $W^{(m)}$ - Algorithm
      implicit real (a - h, o - z)
      parameter(mdim=6, ldim=50, epsdiv=10-77)
      parameter (np=2, m=2, lmax=20, incr=1, sigma=1.3)
      dimension g(mdim), psiai(0:ldim, 2, 2), bigpsi(0:ldim, mdim, 2)
      dimension psig(0:mdim, 2:mdim+1, 2), approx(0:ldim, 0:ldim)
      external mltag
```

```

common /sigkap/sigmap, kappap
common /np/npp/theta/theta
common /rl/irl(0:ldim)
write(6,111)
111 format( 'summation of cf(I)/ limit of Post-Widder sequence')
npp=np
theta=1.q0
sigmap=sigma
kappap=kappa
call wmalgm(mdim, ldim, m, lmax, mltag, g, psiai, bigpsi, psig,
+ approx, epsdiv)
write(6,121)
121 format(/, 3x, 'l', 3x, 'r.l', 3x, 'error(l,0)', 3x, 'error(0,l)')
do l=0, lmax
er1=approx(l,0)
er2=approx(0,l)
write(6,131) l, irl(l), er1, er2
enddo
131 format(2i4, d25.16)
stop
end

```

```

subroutine wmalgm(mdim, ldim, m, lmax, mltag, g, psiai, bigpsi, psig,
+ approx, epsdiv)
implicit real (a - h, o - z)
integer cur, temp, p, pm, q, qp
dimension g(mdim), psiai(0:ldim, 2, 2)
dimension bigpsi(0:ldim, mdim, 2), psig(0:mdim, 2:mdim+1, 2)
dimension approx(0:ldim, 0:ldim)
cur=1
temp=2
call mltag(m, 0, t, a, g)
approx(0, 0)=a
psiai(0, 1, cur)=a/g(1)
psiai(0, 2, cur)=1.0/g(1)
bigpsi(0, 1, cur)=1.0/t
do k=2, m
psig(0, k, cur)=g(k)/g(1)
enddo

```

```

psig(0, m+1, cur)=t
do 80 l=1, lmax
call mltag(m, l, t, a, g)
approx(l, 0)=a
psiai(0, 1, temp)=a/g(1)
psiai(0, 2, temp)=1.0/g(1)
bigpsi(0, 1, temp)=1.0/t
do k=2, m
psig(0, k, temp)=g(k)/g(1)
enddo
psig(0, m+1, temp)=t
sign=-1.0
do 60 p=1, l
if (p.le.m) then
d=psig(p-1, p+1,temp)-psig(p-1, p+1, cur)
do i=p+2, m+1
psig(p, i, temp)=(psig(p-1, i, temp)-psig(p-1, i, cur))/d
enddo
end if

if (p.lt.m) then
bigpsi(p, p+1, temp)=sign/psig(p, m+1, temp)
sign=-sign
end if
pm=min0(p-1, m-1)
do q=1, pm
ps=bigpsi(p-2, q, cur)
dq=ps/bigpsi(p-1, q, cur)-ps/bigpsi(p-1, q, temp)
qp=q+1
bigpsi(p, qp, temp)=(bigpsi(p-1, qp, temp)-bigpsi(p-1, qp, cur))/dq
enddo
if (p.gt.m) then
ps=bigpsi(p-2, m, cur)
d=ps/bigpsi(p-1, m, cur)-ps/bigpsi(p-1, m, temp)
end if
bigpsi(p, 1, temp)=(bigpsi(p-1, 1, temp)-bigpsi(p-1, 1, cur))/d
do i=1, 2
psiai(p, i, temp)=(psiai(p-1, i, temp)-psiai(p-1, i, cur))/d
enddo

```

```

60   continue
      do 70 p=1, l
          j=l-p
          if (abs(psiai(p, 2, temp)).ge.epsdiv) then
              approx(j, p)=psiai(p, 1, temp)/psiai(p, 2, temp)
          else
              approx(j, p)=1075
          write(6,101)j, p
101  format(1x, 'approx(', i3, ',', i3, ') is not defined')
          end if
70   continue
      jj=cur
      cur =temp
      temp=jj
80   continue
      return
      end

```

```

subroutine mltag(m, l, t, a, g)
implicit real(a-h, o-z)
real kappa
parameter(ldim=50)
dimension g(m)
common /sigkap/sigma, kappa
common /rl/irl(0:ldim)

```

```

if (sigma.eq.1.0) then
  lsum=kappa*l+10-10
  lsum=kappa*(l+1)+10-10
end if
if (sigma.gt.1.0) then
  if(l.eq.0) then
    lsum=0
  lsum=1
  else
    lsum=1
  lsum=1
  lsum=1
  do i=1, l
  do i=0, lsum

```

```

ir= sigma*lsum+10-10
if (ir.le.lsum) then
lsum=lsum+1
else
lsum=ir
end if
if (i.eq.l-1)lsump=lsum
enddo
end if
end if
irl(l)=lsum
if (l.eq.0) a=0
do i=lsump+1, lsum
a=a+cf(i)
enddo
p=lsum
t=1.0/p
do k=1, m
g(k)=cf(lsum+k-1)
enddo
do i=2, m
do j=m, i, -1
g(j)=g(j)-g(j-1)
enddo
enddo
do k=1, m
g(k)=g(k)*p
p=p*lsum
enddo
do k=1, m/2
st=g(k)
g(k)=g(m-k+1)
g(m-k+1)=st
enddo
return
end

```

```

function cf(I)
implicit real(a - h, o - z)

```

```

common /np/np/theta/theta
a=float(i)
if (np.eq.1) cf=1.0/a**1.5+2.0/a**2
if (np.eq.2) cf=cos(a*theta)/a
if (np.eq.3) then
t=10.0
c value of t for which inverse transform is required
b=-(a+1.0)
a1=a-1
b1=-(a+1)
if (i.gt.1) goto 150
cf=(1.0+(t/a))**b
goto 100
150 cf=(1+(t/a))**b-(1+(t/a1))**b1
100 end if
if (np.eq.4)then
t=2.0
s=a/t
v=s*s+1
w=1.0/sqrt(v)
z=-(s*w)/v
s1=(a-1)/t
v1=s1*s1+1
w1=1.0/sqrt(v1)
z1=-(s1*w1)/v1
if (i.gt.1) goto 200
cf=-s*s*z
goto 250
200 b=1.0
do j=1, i-1
b=j*b
enddo
do j=2, i
y=-((2*j-1)*s*z+(j-1)*(j-1)*w)/v
w=z
z=y
enddo
if (i.gt.2) goto 300
y1=z1

```

```
      goto 350
300   do j=2, i-1
      y1=-((2*j-1)*s1*z1+(j-1)*(j-1)*w1)/v1
      w1=z1
      z1=y1
      enddo
350   cf=(-((-s)**(a+1))/(a*b))*y+((-s1)**a/b)*y1
250   end if
      return
      end
```

### Program for Crump's Method

Crump's method consists of the application of the epsilon algorithm to the summation in Durbin's Fourier series approximation

$$f(t) \approx \frac{e^{ct}}{T} \left[ \frac{1}{2} \Re \{ \bar{f}(c) \} + \sum_{k=1}^{\infty} \Re \left\{ \bar{f} \left( c + \frac{ik\pi}{T} \right) \right\} \cos \left( \frac{k\pi t}{T} \right) - \sum_{k=1}^{\infty} \Im \left\{ \bar{f} \left( c + \frac{ik\pi}{T} \right) \right\} \sin \left( \frac{k\pi t}{T} \right) \right]$$

See reference, Crump [2].

#### Entry/Exit parameters

1. FUN — a subroutine which evaluates the real and imaginary parts of  $\bar{f}(s)$  (see sample program). This must be declared as external in the program which calls C06LAF.
2. n — integer. n signifies the number of points at which the inverse Laplace transform is required.
3. t(n) — **real** array. On entry  $0.0 \leq t(1) < t(2) < \dots < t(n)$  and the t(j) represent the points at which  $f(t)$  is to be determined.
4. valinv(n) — **real** array. On exit gives an estimate for  $f(t)$  for each  $t(j)$ .
5. errest(n) — **real** array. On exit gives an estimate for the relative errors of the components in valinv(n). If valinv(j) < relerr, then errest(j) estimates absolute error.
6. relerr — **real**. On entry the required relative error in the values of the inverse Laplace transform.
7. alphab — **real**. An upper bound for  $c$ . Ideally it should equal  $c$  or be slightly larger. If it is less than  $c$  the prescribed accuracy might not be attained.
8. tfac — **real**. On entry a factor to be used in calculating the value of  $T$ . The suggested value of tfac is **0.8** but it must be greater than **0.5**.
9. mxterm — integer. On entry the maximum number of terms used in the evaluation of the Fourier series. It is suggested that  $\text{mxterm} \geq 100$ . Certainly  $\text{mxterm} \geq 1$ .
10. nterms — integer. On exit gives the number of terms of the Fourier series actually used.
11. na — integer. The number of values of  $c$  used by the routine.
12. alow/ahigh - **real**. Respectively the lowest and highest values values of  $c$  used in the algorithm. These can be used for checking

alphab.

13. nfeval — integer. On exit records the number of calls made to the subroutine FUN.

14. work(4\*mxterm+2) — **real** array. used as working space.

15. ifail — integer. On entry ifail must be set to 0, -1 or 1. On exit ifail = 0 unless the routine detects an error. See the NAG Library specification for more details regarding error indications.

The NAG Library specification should also be consulted for further details on Accuracy and the choice of alphab and other precautions which are advised.

```
c      Program for Crump's method
c      Uses NAG Library routine C06LAF
      integer nmax, mxterm, nout
      parameter (nmax=20, mxterm=500, nout=6)
      real ahigh, alow, alphab, relerr, tfac
      integer i, ifail, n, na, nfeval, nterms
      real errest(nmax), t(nmax), valinv(nmax), work(4*mxterm+2)
      external C06LAF, FUN

      read(5,*)n
      do i=1, n
      read(5,*)t(i)
      enddo

      write(nout,*)'alphab=?'
      read(5,*)alphab
      write(nout,*)'relerr=?'
      read(5,*)relerr
      write(nout,*)'tfac=?'
      read(5,*)tfac
      write(nout,*)
      write(nout,999)'mxterm=', mxterm, 'tfac=', tfac,
+ 'alphab=', alphab, 'relerr=', relerr
      ifail=-1

      call C06LAF(FUN, n, t, valinv, errest, relerr, alphab, tfac, mxterm,
+ nterms, na, alow, ahigh, nfeval, work, ifail)
```

```

if(ifail.gt.0 .and. ifail.lt.5)goto 60
write(nout,*)
write(nout,*) '          t          result          '

do i=1, n
write(nout,998) t(i), valinv(i)
enddo
write(nout,997)'nterms=', nterms,   'nfeval=', nfeval,
+ 'alow=', alow,   'ahigh=', ahigh,   'ifail=', ifail

c    test for larger values of c

relerr=1.0-3
tfac=0.8
write(nout,*)
write(nout,999)'mxterm=', mxterm,   'tfac=', tfac,
+ 'alphan=', alphan,   'relerr=', relerr
ifail=-1
call C06LAF(FUN, n, t, valinv, errest, relerr, alphan, tfac, mxterm,
+ nterms, na, alow, ahigh, nfeval, work, ifail)

if (ifail.gt.0 .and. ifail.lt.5)goto 60

write(nout,*)
write(nout,*) '          t          result          '
do i=1, n
write(nout,998) t(i), valinv(i)
enddo
60  write(nout,*)
write(nout,997)'nterms=', nterms,   'nfeval=', nfeval,
+ 'alow=', alow,   'ahigh=', ahigh,   'ifail=', ifail

999  format(1x, a, i4, a, f6.2, a, f6.2, a,1p, d8.1)
998  format(1x, f4.1, 7x, f9.6)
997  format(1x, a,i4, a, i4, a, f7.2, a, f7.2, a, i2)
stop
end

subroutine FUN(pr, pi, fr, fi)

```

```

c      evaluates  $f(s) = 1/\sqrt{(s^2 + 1)}$ 
      real pr, pi, fr, fi, zr, zi
      external A02AAF
c      NAG routine A02AAF evaluates the square root of a complex number
      external A02ACF
c      NAG routine A02ACF evaluates the inverse of a complex number
      fr=pr*pr-pi*pi+1.0
      fi=2.0*pr*pi
      call A02AAF(fr, fi, zr, zi)
      call A02ACF(1.0, 0.0, zr, zi, fr, fi)
      return
      end

```

## Program for Post-Widder method

This program applies the rho-algorithm to extrapolate the Post-Widder sequence. An odd number of terms are required to be calculated.

### Entry/Exit Parameters.

1.  $m$  — integer variable. In the example provided below if  $m=1$  then the inverse transform of  $\bar{f}(s) = 1/(s+1)$  is found while  $m=2$  will give the inverse transform for  $\bar{f}(s) = 1/\sqrt{(s^2+1)}$ .
2.  $n$  — integer variable. The number of terms to be used in the rho algorithm.  $n$  must be odd and a maximum of 45.
3.  $t$  — **real** variable. The value of  $t$  at which the inverse transform is required.
4.  $\text{rho2}$  — a **real** array. The contents of the array are the  $n$  terms of the Post-Widder sequence. The routine which calculates the sequence must be provided by the user.

Each cycle of the rho-algorithm will be printed out and the final result printed will give the estimate for  $f(t)$ . The accuracy of the estimate can be gauged by comparing with the alternate cycle which precedes it.

```
      real rho1(45),rho2(45),a,b,c,d
      read(5,*)m
c     m indicates the sequence to be computed
c     m=1,  $\bar{f}(s) = 1/(s+1)$ ;  m=2,  $\bar{f}(s) = 1/(s^2+1)^{1/2}$ 
      read(5,*)n
c     n must be odd,  $n \leq 45$ 
      call rhoalg(m, n)
      stop
      end

      subroutine rhoalg(m, n)
      real rho1(45), rho2(45), a
      do i=1, n
      rho1(i)=0
      enddo
      if (m.eq.1) goto 50
      call sequence2(n, rho2)
```

```

      goto 100
50    call sequence1(n, rho2)
100   do k=1, n-1
      do i=1, n-k
        rho1(i)=rho1(i+1)+float(k)/(rho2(i+1)-rho2(i))
        write(6,*)rho1(i)
      enddo
      write(6,*)'new cycle'
      do i=1, n-k
        a=rho1(i)
        rho1(i)=rho2(i)
        rho2(i)=a
      enddo
    enddo
  return
end

subroutine sequence1(n, x)
  real x(45), t, a, b
  read(5,*)t
  do i=1, n
    a=float(i)
    b=-(a+1)
    x(i)=(1+(t/a)**b)
    write(6,*)x(i)
  enddo
  return
end

subroutine sequence2(n, x)
  real x(45), u(0:45), t, a, b, f, s, v, w
  v=-1.0
  w=1.0
  read(5,*)t
  do i=1, n
    a=float(i)
    b=a+1
    s=a/t
    w=w*v
  enddo

```

```

x(i)=w*(s)**b
call fac(i,f)
x(i)=x(i)/f
call deriv(i,s,u)
x(i)=x(i)*u(i)
write(6,*)x(i)
enddo
return
end

```

```

subroutine fac(i, f)
real f
f=1.0
do j=1, i
f=j*f
enddo
return
end

```

```

subroutine deriv(i, s, u)
real r, s, t, u(0:45)
t=s*s+1
u(0)=1.0/sqrt(t)
u(1)=-(s/t)*u(0)
if (i.eq.1) goto 100
do j=2, i
r=float(j)
u(j)=(2*r-1)*s*u(j-1)+(r-1)*(r-1)*u(j-2)
u(j)=-u(j)/t
enddo
100 return
end

```

## Program for the Honig-Hirdes method for Laplace Inversion

This program is based on the Durbin approach to evaluating the inverse Laplace transform but differs from the Crump method by applying the Korrektur technique of Albrecht and Honig to reduce the discretization error.

### Entry/Exit Parameters.

1.  $f$  — a **real** subroutine which evaluates  $\bar{f}(s)$  given **real** parameters  $sr(= \Re s)$  and  $si(= \Im s)$  the results being indicated by the **real** parameters  $fr(= \Re \bar{f}(s))$  and  $fi(= \Im \bar{f}(s))$ . This subroutine must be declared as external and supplied by the user.
2.  $t1, tn$  — **real** parameters which are respectively lower and upper bounds of the interval in which  $f(t)$  is to be approximated.
3.  $n$  — integer variable, the number of values  $t_k, k = 1, \dots, n$  at which  $f(t)$  is to be computed. Note that

$$t_k = t1 + (tn - t1)k/(n + 1),$$

so that if we require  $t_k = 10 + k, k = 1, \dots, 10$  we have to set  $t1=10$  and  $tn=21$ .

4.  $iman$  — integer variable. If it is set to 0 all further parameters are set automatically (except  $ns1$  which has to be 60). If it is 1 a manual choice of the parameters  $ilapin, ikonv, ns1, ns2, icon, ikor, con$  is possible. In the example below  $iman=0$ .
5.  $ilapin$  — integer variable. If  $ilapin = 1$  the approximation formula is applied at  $T = t$  while if  $ilapin = 2$  it is applied at  $T=tn$  (or  $2tn$  for the Korrektur terms).
6.  $ikonv$  — integer. If  $ikonv=1$  the minimum-maximum method is invoked while  $ikonv=2$  invokes the  $\epsilon$  - algorithm.
7.  $ns1$  — integer. The number of function evaluations of  $\bar{f}(s)$  which are used in order to estimate  $f(t)$ .  $ns1=60$  if  $iman=0$ .
8.  $ns2$  — integer. The number of function evaluations of  $\bar{f}(s)$  used to approximate the Korrektur term.
9.  $icon$  — integer. If  $icon=0$  then there is no optimal choice of free parameters. If  $icon = 1$  then there is optimal choice of free parameters for  $t = t_{[n/2]}$  while if  $icon=2$  there is optimal choice of free parameters for  $t = t_k$ .
10.  $ikor$  — integer. If  $ikor = 0$  there is no application of the Korrektur method otherwise it is 1.

11. `con` — **real**. If `icon = 0` then the free parameter  $c$  is determined from  $con = cT$ .
12. `h(6,n)` — a **real** array which on exit contains  $f(t_k)$  in row 1. The second row is a work area. The third row contains the computed optimal parameter  $con_{opt} = c_{opt} \cdot T$  for  $t = t_k$ . The fourth row gives the code for the acceleration method adopted (0 — no acceleration of convergence, 1 — minimax, 2 — epsilon algorithm(`epal`), 4 — curve fitting method(`cfm`),  $P = ns1+2$  — indicates overflow in `epal` if  $P \geq 4$ ). The fifth row contains the absolute error calculated by formula (33) in the Honig - Hirdes paper and the sixth row contains a control number of up to 6 digits which is explained in Honig and Hirdes [6].
13. `E(3,ns1)` — a **real** array used as working space.
14. `iout` — integer. Refers to the output device used.
15. `ier` — integer. Parameter which indicates error in the input data. If `ier = 0` there is no error. Otherwise the error is indicated by the print-out.

```

integer n, iman, ilapin, ikonv, ns1, ns2, icon, ier, iout
parameter (n=10, ns1=60, iman=0)
real t1, tn, con, h(6,n), e(3,ns1)
external f
read(5,*)t1, tn
iout=6
call lapin(f, t1, tn, n, iman, ilapin, ikonv, ns1, ns2, icon, iker,
+ con, h, e, ier, iout)
do i=1,n
t=t1+(tn-t1)*i/(n+1)
write(iout,*)t, h(1,n)
enddo
stop
end

subroutine lapin(f, t1, tn, n, iman, ilapin, ikonv, ns1, ns2, icon,
+ iker, con, h, e, ier, iout)

real abrn, absf, con, conopt, con1, con2, del, e, fn, fns1
real freal, fimag, h, pi, racc, rnsun, rnsunk, t, ta, tb
real tk, tn, t0, t1, v1, v2, w

```

```

integer hmono
external f
dimension h(6,n), e(3,ns1)
common /clapin/ ta, tb, t0, conopt, absf, lval, hmono

c   initialise array h
do i=1, n
do j=1, 6
h(j,i)=0.0
enddo
enddo

ier=0
if (tn.lt.t1) ier=1
if (n.lt.1) ier=ier+10
if (iman.eq.0) goto 100
if (iman.eq.1) goto 110
ier=ier+100
goto 120

c   parameters for iman=0
100 if (ns1.ne.60) ier=ier+100000
if (ier.ne.0) goto 120
ilapin=1
ikonv=2
icon=1
ikor=0
ns2=0
goto 200

c   iman=1
110 if (ilapin.lt.1 .or. ilapin.gt.2) ier=ier+1000
if (ikonv.lt.1 .or. ikonv.gt.2) ier=ier+10000
if (ns1.lt.1 .or. (ns2.lt.1 .and. ikor.eq.1)) ier=ier+100000
if (icon.lt.0 .or. icon.gt.2 .or. (icon.eq.2 .and. ilapin.eq.2))
+ ier=ier+1000000
if (ikor.lt.0 .or. ikor.gt.1) ier=ier+10000000
if (icon.eq.0 .and. con.le.0.0) ier=ier+100000000
if (ier.eq.0)goto 200

```

```

120  call error(ier, t1, tn, n, iman, ilapin, ikonv, ns1, ns2, icon,
+    ikor, con, iout)
    return

200  pi=4.0*atan(1.0)
    con1=20.0
    con2=con1- 2.0
    absf=0.0

    j3=(3-icon)/2 + n*(icon/2)
    ta=t1
    tb=tn
    do 830 l3=1, j3
    lval=l3
    hmono=0
    kor1=ikor

c    computation of the optimal parameters
210  if (icon-1) 215,230,220
215  jump=0
    call lapin2(f, t1, tn, n, ilapin, ikonv, ns1, ns2, icon, ikor, con, h, e, jump)
    goto 830
220  ta=t1+float(l3)*(tn-t1)/float(n+1)
    tb=ta
230  nh=n/2
    t=ta+(tb-ta)*float(nh)/float(n+1)
    tk=float(2-ilapin)*t+float(ilapin-1)*tb

c    computation of the truncation error (rnsun)
    t0=t
    con =con1
    jump=1
    call lapin2(f, t1, tn, n, ilapin, ikonv, ns1, ns2, icon, ikor, con, h, e, jump)
240  fn=h(1,13)
    fns1=e(1,ns1)
    con=con2
    jump=2
    call lapin2(f, t1, tn, n, ilapin, ikonv, ns1, ns2, icon, ikor, con, h, e, jump)
250  if (fn.ne.h(1,13) .and. fns1.ne.e(1,ns1))goto 255

```

```

conopt=con
absf=0.0
goto 320
255 rnsu=tk*(fn-h(1,l3))/exp(con1)-exp(con2)
if (ilapin.eq.2)goto 260

c computation of the acceleration factor (del)
racc=t*(fns1-e(1,ns1))/(exp(con1)-exp(con2))
del=rnsu/racc

260 if (ikor.eq.1)goto 280

c optimal parameters (Method A)
t0=2.0*tk+t
con=con1/4.0
jump=3
call lapin2(f, t1, tn, n, ilapin, ikonv, ns1, ns2, icon, ikor, con, h, e, jump)
270 fn=h(1,l3)
conopt=-tk/(2.0*tk+t)*log(abs(rnsu/(tk*fn)))
goto 310

c optimal parameters for the Korrektur method (Method A)
280 t=4.0*tk+t
con=con1/4.0
jump=4
call lapin2(f, t1, tn, n, ilapin, ikonv, ns1, ns2, icon, ikor, con, h, e, jump)
290 fn=h(1,l3)
t0=8.0*tk+t
jump=5
call lapin2(f, t1, tn, n, ilapin, ikonv, ns1, ns2, icon, ikor, con, h, e, jump)
300 fn=fn-h(1,l3)
conopt=-tk/(4.0*tk+t)*log(abs(rnsu/(tk*fn)))

c optimal parameters (Method B)
310 if (ilapin.eq.1)goto 315
absf=abs(exp(conopt)*rnsu*2.0/tk)
goto 320
315 v1=con1/t
v2=conopt/t

```

```

w=pi*float(ns1)/t
call f(v2, w, freal, fimag)
rnsstk=rnsstk*freal
call f(v1, w, freal, fimag)
rnsstk=rnsstk/freal
abrns=(rnsstk-rnsstk)/(v2-v1)
conopt=-log( abs(abrn/t+rnsstk)/(t*float(ikor*2+2)*fn)))/
+ float(3+2*ikor)
v1=v2
v2=conopt/t
call f(v2, w, freal, fimag)
rnsstk=rnsstk/freal
absf=exp(conopt)/t*abs(rnsstk)+
+ abs(exp(-2.0*conopt)*fn*float(ikor-1))
+ exp(-4.0*conopt)*fn*float(ikor))

320 if (conopt.le.0.0) conopt=1.0
jump=6
call lapin2(f, t1, tn, n, ilapin, ikonv, ns1, ns2, icon, ikor, con, h, e, jump)
830 continue
return
end

subroutine lapin2(f, t1, tn, n, ilapin, ikonv, ns1, ns2, icon, ikor,
+ con, h, e, jump)
c Laplace inversion with optimal parameters

real a, absf, b, con, conopt, delta, divi, e, e1, e2, e3, eins
real faktor, fimag, freal, h, pi, pit, pite, ral, suim, sure
real ta, tb, te, tl, tm, tm1, tn, tt, t0, t1, x1, x2, x3, v, w, y1, y2, y3
integer richt, richta, hmono
external f
dimension h(6,n), e(3,ns1), e3(3)
common /clapin/ ta, tb, t0, conopt, absf, l3, hmono

pi=4.0*atan( 1.0)
if (jump.eq.0) goto 360
if (jump.lt.6) goto 370

```

```

t0=ta
tt=tb
i1=l3
j1=(2-icn)*n+(icn-1)*l3
con=conopt
kor1=ikor
goto 380

360  t0=t1
      tt=tn
      i1=1
      j1=n
      kor1=ikor
      jump=6
      goto 380
370  kor1=0
      tt=t0
      i1=l3
      j1=l3

380  delta=(tt-t0)/float(n+1)
      nsum=ns1

c    computation of the t-values from t0, tt
do 805 k2=1, 2
if (ilapin.eq.1) goto 420
te=float(k2)*tt
v=con/te
call f(v, 0.0, freal, fimag)
ral=-0.5*freal
pite=pi/te

405  do l=1, nsum
      w=float(l-1)*pite
      call f(v, w, freal, fimag)
      e(2,l)=freal
      e(3,l)=fimag
      enddo

```

```

420  do 800 k1=i1, j1

      tl=t0+float(k1)*delta
      if (ilapin.eq.2) goto 440

      if (k2.eq.2) tl=3.0*tl
      v=con/tl
      faktor=exp(v*tl)/tl
      call f(v,0.0,freal,fimag)
      ral=-0.5*freal
      pit=pi/tl
      eins=1.0
      sure=0.0

c     method of Durbin
425  do l=1, nsum
      w=float(l-1)*pit
      call f(v, w, freal, fimag)
      sure=sure+freal*eins
      eins=-eins
      e(1,l)=faktor*(ral+sure)
      enddo
      goto 460

440  if (k2.eq.2) tl=tl+te
      faktor=exp(v*tl)/te
      sure=0.0
      suim=0.0
      do l=1, nsum
      w=float(l-1)*pite
      sure=sure+e(2,l)*cos(w*tl)
      suim=suim+e(3,l)*sin(w*tl)
      e(1,l)=faktor*(ral+sure-suim)
      enddo

c     search for stationary values
460  nmax=nsum*2/3
      monoto=0
      k=0

```

```

richta=sign( 1.5,(e(1,nsum)-e(1,nsum-1)))
do l=1, nmax
j=nsum-1
richt=sign( 1.5,e(1,j)-e(1,j-1)))
if (richt.eq.richta) goto 500
k=k+1
e3(k)=e(1,j)
richta=richt
if (k.eq.3) goto 510
500 enddo
if (k.eq.0) goto 700
h(k2, k1)=e(1, nsum)
if (k2.eq.1) h(4, k1)=0
goto 790
510 ke=2
if ((e3(ke)-e(1,j))*float(richta).gt.0) goto 560
jmin=nsum/3
jmax=j-1
do jj=jmin, jmax
j=j-1
richt=sign(1.5, (e(1, j)-e(1, j-1)))
if (richt.eq.richta) goto 540
richta=richt
ke=3-ke
if ((e3(ke)-e(1, j))*float(richta).gt.0.0)goto 560
540 enddo
550 monoto=1
if (ikonv.eq.2) goto 630

c    minimum-maximum method (minimax)
560 h(k2, k1)=(e3(1)+e3(3))/4.0+e3(2)/2.0
if (k2.eq.1) h(4, k1)=1
goto 790

c    epsilon algorithm (epal)
630 k=0
nsumm1=nsum-1
e2=e(1, 1)
do l=1, nsumm1

```

```

e1=e(1,1)
tm=0.0
lp1=l+1
do m=1, l
mm=lp1-m
tm1=e(1, mm)
divi=e(1, mm+1)-e(1, mm)
if (abs(divi).gt.1.0-20) goto 640
k=1
goto 670
640 e(1, mm)=tm+1.0/divi
tm=tm1
enddo
e2=e1
enddo

670 if ( abs(e1).gt.abs(e2) e1=e2
if ( abs(e(1,1)).gt.abs(e1)) e(1, 1)=e1
h(k2, k1)=e(1, 1)
if (k2.eq.1) h(4, k1)=k+2
goto 790

c curve fitting (cfm)
700 x1=float(nsum)-2.0
x2=float(nsum)-1.0
x3=float(nsum)-0.0
y1=e(1, nsum-2)
y2=e(1, nsum-1)
y3=e(1, nsum)
b=((y3-y1)*x3*x3*(x1+x2)/(x1-x3)
+ (y2-y1)*x2*x2*(x1+x3)/(x1-x2))/(x3-x2)
a=((y2-y1)-b*(x1-x2)/(x1*x2))*(x2*x2*x1*x1)/(x1*x1-x2*x2)
h(k2,k1)=y1-(a/x1+b)/x1
monoto=1
if (k2.eq.1) h(4, k1)=3

790 h(3, k1)=con
h(5, k1)=absf
hmono=hmono+k2*monoto*10**(6-jump)

```

```

      if (jump.lt.6) goto 800
      h(6, k1)=float((2-k2)*hmono+
+ float(k2-1)*(float(2*monoto)+h(6, k1))
      hmono=hmono/10*10

800  continue
      if (kor1.eq.0) return
      if (k2.eq.2) goto 810
      nsum=ns2
805  continue

c    Korrektur method
810  faktor=-exp(-2.0*con)
      do k=i1, j1
      h(1, k)=h(1, k)+faktor*h(2, k)
      enddo

      return
      end

      subroutine error(ier, t1, tn, n, iman, ilapin, ikonv, ns1, ns2, icon, ikor,
*      con, iout)
      real t1, tn, con
      write(iout,1)ier, t1, tn, n, iman, ilapin, ikonv, ns1, ns2, icon, ikor, con
1    format(///14h *** error ***, 8x, 5hier =, i12//
*    10h t1 * , d10.3, 18x, 12h1 * tn < t1/
*    10h tn * , d10.3/
*    10h n * , i10, 17x, 11h10 * n < 1/
*    10h iman * , i10, 16x, 29h100 * iman < 0 or iman > 1/
*    10h ilapin * , i10, 15x, 34h1000 * ilapin < 1 or ilapin > 2/
*    10h ikonv * , i10, 15x, 33h10000 * ikonv < 1 or ikonv > 2/
*    10h ns1 * , i10, 13x, 38h100000 * ns1 < 1 or (ns2 < 1 and ,
*    41hikor = 1) or (ns1 <> 60 and iman = 0)/
*    10h ns2 * , i10/
*    10h icon * , i10, 12x, 36h1000000 * icon < 0 or icon > 2 or,
*    29h (icon = 2 and ilapin = 2)/
*    10h ikor * , i10, 11x, 34h10000000 * ikor < 0 or ikor > 1/
*    10h con * , d10.3, 10x, 21h100000000 * con <= 0//)
      return

```

```
end  
  
c  subroutine f(sr, si, fr, fi)  
   evaluates function  $1/(s^2 + 1)$   
   real sr, si, fr, fi, a  
   fr=sr*sr-si*si+1.0  
   fi=2*sr*si  
   a=fr*fr+fi*fi  
   fr=fr/a  
   fi=-fi/a  
   return  
end
```

### Program for Talbot's method

This is a sub-program of Algorithm 682 by Murli and Rizzardi [8]. It omits a section of the Murli-Rizzardi program which deals with essential singularities. Readers should be warned that some of the variable names used by Murli and Rizzardi have been changed to be more consistent with the values used in the text and in the original Talbot paper. Examples are conlam, consig, and connu and tvalue which have become lam, sig, nu and tval.

#### Entry/Exit parameters

1. flap — a **complex** subroutine which evaluates  $\bar{f}(s)$  for complex arguments. This subroutine must be supplied by the reader.
2. finv — a **real** function which evaluates the function  $f(t)$  at the given data points for some known test function. This will give a measure of confidence when operating the program with  $f(t)$  unknown. In this situation take  $f(t)$  equal to **1.0**.
3. sings — this routine must return the number of singularities, their location and multiplicity. There is a restriction as the number of singularities may not exceed 24.
4. nt — integer. The number of data points at which the Laplace transform is required.
5. vt — **real** array of dimension nt. Data to be supplied by the user. In the example below data values are **0.5, ..., 64.0**.
6. nosing — integer. The number of singularities of the function  $\bar{f}(s)$  with non-negative imaginary parts.
7. singre — real array of dimension  $\leq 24$ . This array contains the real parts of the singularities.
8. singim — real array of dimension  $\leq 24$ . This array contains the imaginary parts of the singularities.
9. multsi — integer array. This array records the multiplicity of each singularity.  
For example, if  $\bar{f}(s) = 1/(s-1)^3[(s-0.5)^2 + 4]$ , we would set  
nosing=3,  
singre(1)=1, singim(1)=0, multsi(1)=2;  
singre(2)=0.5, singim(2)=2, multsi(2)=0;  
singre(3)=0.5, singim(3)=-2, multsi(3)=0;  
in the subroutine sings.
10. invf — **real**. The computed value of  $f(t)$ .
11. nopts — integer. The number of points used in the Talbot summation as computed by the subroutine tapar.

12. `ic` — integer. The machine decimal precision used by Talbot's method.
- 12a. `id` — an integer between 1 and `ic+2`.
13. `ier` — integer. This is an error indicator. `ier=0` indicates normal termination. `ier =1` indicates that the output value of the subroutine `finv` causes overflow and a scaled value of  $f(t)$  is returned.
14. `pserr` — real. This is the ratio of absolute error/ $(e^{\sigma t})$ .
15. `error` — real. This is the relative (R) error when the value produced by `finv` is greater than 1. Otherwise it is the absolute error (A).

```

implicit real(a-h, o-z)
real lam, nu, invf
real finv, fv, tt, error, pserr, dinvf, demax, d2mach
real r1mach(3), r1
c   the machine constants r1mach(*) are defined by Murli and Rizzardi
c   — this program gives the IEEE 754 specification for these constants
external flap
complex flap
character*1 alfa
dimension singre(24), singim(24), multsi(24), vt(8)
data ndim/24/
data vt/0.5, 1.0, 2.0, 4.0, 8.0, 16.0, 32.0, 64.0/
data d2mach/Z'7fefeffeffeffeff' /
c   d2mach is the double length version of r1mach(2)
data r1mach(2)/Z'7f7fffff' /
data r1mach(3)/Z'33800000' /
nt=8
ic=-ifix(log10(r1mach(3))*3./4.)
demax=log(d2mach)
emax=log(r1mach(2))
call sings(ndim, singre, singim, multsi, nosing)
write(6,200)(singre(k), singim(k), multsi(k), k=1, nosing)
do 2 it=1, nt
tval=vt(it)
tt=dble(tval)
if (tval.gt.demax) then
    fv=0.0

```

```

else
    fv=finv(tval)
endif
if (abs(fv).gt.1.0) then
    alfa='R'
else
    alfa='A'
endif

do 3 id=1, ic+2
call tapar(tval, id, nosing, singre, singim, multsi, ic,
*   lam, sig, nu, nopts)
if (id.eq.1) then
    if (tval.gt.demax) then
        write(6,*)tval, lam, sig, nu
    else
        write(6,*)tval, lam, sig, nu, fv
    endif
endif

call tsum(flapp, lam, sig, nu, nopts, tval, invf, ier)
if (ier.eq.0) then
    pserr=(fv-invf)/exp(tt*sig)
    if (alfa.eq.'R') then
        error=(fv-invf)/fv
    else
        error=fv-invf
    endif
write(6,*)id, nopts, invf, pserr, error, alfa
else
    write(6,*)id, nopts, invf, ier
if (tval.gt.emax.and.tval.lt.demax) then
    dinvf=lam/nopts*exp(tt*sig)*invf
    pserr=(fv-dinvf)/exp(tt*sig)
    error=(fv-dinvf)/fv
    write(6,*)dinvf, pserr, error, alfa
endif
endif
endif
3 continue

```

```

2      continue
      stop
200    format('singularities and their multiplicities'/
*      (2(2x, e12.6), 2x, I2))
      end

      subroutine tapar(tval, decdig, nosing, singre, singim, multsi, ic,
*      lam, sig, nu, nopts)
c      This subroutine evaluates the geometrical parameters
c      lam(bda), sig(ma) and nu for the Talbot contour and the
c      accuracy parameter (nopts)
      implicit real (a-h, o-z)
      real lam,nu
      real pi
      logical caso1
      integer ic, decdig, dd
      dimension singre(nosing), singim(nosing), multsi(nosing)

      data pi/0.0/
      if (pi.eq.0.0) pi=4.*atan(1.0)
      caso1=.true.
      omega=0.4*(ic+1)

      sig0=0.0
      pmax=singre(1)
      kmax=1
      if (nosing.eq.1) goto 3
      do j=1, nosing
      if (singre(j).gt.pmax) pmax=singre(j)
      if (multsi(j).gt.multsi(kmax)) kmax=j
      enddo
3      if (pmax.gt.sig0) sig0=pmax

      rd=0.0
      sid=0.0
      tetd=pi
      do 7 j=1, nosing
      if (singim(j).le.0.0) goto 7
      caso1=.false.

```

```

    etaj=atan2(-singre(j)+sig0,singim(j))
    tetj=etaj+pi/2.
    rj=singim(j)/tetj
    if (rd.ge.rj) goto 7
    rd=rj
    tetd=tetj
    id=j
7   continue

    if (caso1) goto 8
    srd=singre(id)-sig0
    sid=singim(id)
    md=multsi(id)
    v=sid*tval
    omega=min(omega+v/2.0,2.0*(ic+1)/3.0)
    if (1.8*v.gt.omega*tetd) goto 9

    caso1=.true.
8   lam=omega/tval
    sig=sig0
    nu=1.0
    goto 10
9   caso1=.false.
    pk=1.6+12.0/(v+25.0)
    fi=1.05+1050./max(553.0, 800.0-v)
    pmu=(omega/tval+sig0-pmax)/(pk/fi-1.0/tan(fi))
    lam=pk*pmu/fi
    sig=pmax-pmu/tan(fi)
    nu=sid/pmu

10  n1=0
    e=( 2.3*decdig+omega)/(lam+tval)
    if (e.gt.4.4) goto 11
    unro=( 16.0+4.3*e)/(24.8-2.5*e)
    goto 13
11  if (e.gt.10.0) goto 12
    unro=(50.0+3.0*e)/(129.0/e-4.0)
    goto 13
12  unro=(44.0+19.0*e)/(256.0/e+0.4)

```

```

13   n1=lam*tval*(unro+(nu-1.0)/2.0)
      n1=n1+1
      n0=0
      n2=0

      if (sid.eq.0.0) goto 15
      dd=decdig+2*min(md-1,1)+md/4
      if (.not.caso1.or.(md.eq.0)) goto 14
      p=srd/lam
      q=sid/lam
      call invpc(p, q, tetd, u, pi)
      if (u.le.0.0)goto 14
      n0=(2.3*dd+srd*tval)/u
      n0=n0+1
14   gamm=(sig-sig0)/lam
      y=v/1000.0
      eta=min(1.78,1.236+0.0064*(1.78**dd))
      eta=eta*(1.09-y*(0.92-0.8*y))
      n2=eta*nu*(2.3*dd+omega)/(3.0+4.0*gamm+1.0/exp(gamm))
      n2=n2+1
      nopts=max(n0, n1)
      nopts=max(n2, nopts)
      return

15   dd=decdig+2*min(multsi(kmax)-1,1)+multsi(kmax)/4
      n2=(2.3*dd+omega)/2.0
      n2=n2+1
      icm1=ic-1
      if (dd.lt.icm1) goto 17
      q=0.0
      do 16 l=1, nosing
      if (multsi(l).eq.0) goto 16
      dd=decdig+2*min(multsi(l)-1, 1)+multsi(l)/4
      srd=singre(l)-sig0
      if (.not.(dd.ge.icm1.and.srd.lt.0.0)) goto 16
      p=srd/lam
      call invpc(p, q, tetd, u, pi)
      if (u.le.0.0)goto 16
      n0l=(2.3*dd+tval*srd)/u

```

```

        if (n0l.gt.n0) n0=n0l
16      continue
        n0=n0+1
17      nopts=max(n0, n1)
        nopts=max(n2, nopts)
        return
        end

subroutine tsum(flap, lam, sig, nu, nopts, tval, finv, ier)
c      This routine gives the trapezoidal rule approximation
c      for the inverse Laplace transform
implicit real (a-h, o-z)
real lam, nu
real pi
external flap
complex flap, s, ff
real r1mach(2), r1
data r1mach(1)/Z'00800000'/
data r1mach(2)/Z'7f7fffff'/
data pi/0.0/
elim=log(r1mach(1))
if (pi.eq.0.0) pi=4.0*atan(1.0)
piovn=pi/float(nopts)
ier=0
tau=lam*tval
psi=piovn*tau*nu
c=cos(psi)
br=0
bi=0
dbr=0
dbi=0
nm1=nopts-1
finv=0
if (nm1.eq.0) goto 5

c      Reinsch algorithm
if (c.gt.0) goto 2
c      Case  $\cos(\psi) \leq 0$ 
u=4.0*cos(psi/2)**2

```

```

do k=nm1, 1, -1
theta=k*piovn
alpha=theta*cos(theta)/sin(theta)
beta=theta+alpha*(alpha-1.0)/theta
sr=lam*alpha+sig
si=lam*nu*theta
s=cplx(sr, si)
ff=flap(s)
g=real(ff)
h=imag(ff)
arg=alpha*tau
if (arg.le.elim) then
    eat=0.0
else
    eat=exp(arg)
endif
br=dbr-br
bi=dbi-bi
dbr=u*br-dbr+eat*(g*nu-h*beta)
dbi=u*bi-dbi+eat*(h*nu+g*beta)
enddo
br=dbr-br
bi=dbi-bi
dbr=u*br-dbr
goto 4

c Case cos(psi)>0
2 u=-4.0*sin(psi/2)**2
do k=nm1, 1, -1
theta=k*piovn
alpha=theta*cos(theta)/sin(theta)
beta=theta+alpha*(alpha-1.0)/theta
sr=lam*alpha+sig
si=lam*nu*theta
s=cplx(sr, si)
ff=flap(s)
g=real(ff)
h=imag(ff)
arg=alpha*tau

```

```

    if (arg.le.elim) then
        eat=0.0
    else
        eat=exp(arg)
    endif
    br=dbr+br
    bi=dbi+bi
    dbr=u*br+dbr+eat*(g*nu-h*beta)
    dbi=u*bi+dbi+eat*(h*nu+g*beta)
enddo
br=dbr+br
bi=dbi+bi
dbr=u*br+dbr
c    end of Reinsch algorithm

4    finv=dbr-br*u/2.0-bi*sin(psi)
5    sr=lam+sig
    s=cmplx(sr)
    ff=flap(s)
    g=real(ff)
    finv=(finv+nu*exp(tau)*g/2.0)
    if (finv.eq.0.0) return
    if (finv.gt.0.0) then
        signum=1.0
    else
        signum=-1.0
    endif

    cost=log(r1mach(2))
    of=sig*tval+log(lam*abs(finv)/nopts)
    if (of.gt.cost) then
        ier=1
        write(6,*)'ier=', ier
    else
        finv=exp(of)*signum
    endif
    return
end

```

```

subroutine invpc(p, q, theta, u, pi)
implicit real (a-h, o-z)
r=p*p+q*q
r=sqrt(r)
x=13.0/(5.0-2*p-q-0.45*exp(p))
y=2*pi-x
k=1
100 continue
ang=y-theta
s=sin(ang)
c=cos(ang)
b=q-y
e=-b/s
arg=e/r
if (arg.le.0.0) then
u=-1.0
goto 200
endif
u=log(arg)
g=p+b*c/s+u
dy=b*g/(1.0+e*(e-2.0*c))
if (abs(dy).lt.0.0001) goto 200
if (k.ge.100) goto 200
k=k+1
y=y+dy
goto 100
200 continue
return
end

complex function flap(s)
complex s, a, b, I
flap=log(s)/s
return
end

subroutine sings(ndim, singre, singim, multsi, nosing)
implicit real (a-h, o-z)
dimension singre(ndim), singim(ndim), multsi(ndim)

```

```
nosing=1
singre(1)=0.0
singim(1)=0.0
multsi(1)=0
return
end
```

```
real function finv(t)
real a
write(6,*)'t=', t
a=dbl(e(t)
finv=-0.57721566490153286-log(a)
return
end
```

### Mathematica program for Talbot's method

This program is taken from Abate and Valkó [1]. We reproduce this program and give the results when  $\bar{f}(s) = 1/(s^3 - 8)$  in Chapter 10.

```
FT[F_ , t_ , M_]:=Module[{np, r, S, theta, sigma},
np=Max[M, $ MachinePrecision]; r=SetPrecision[2M/(5t), np];
S=r theta (Cot[theta]+I);
sigma=theta+(theta Cot[theta]-1)Cot[theta];
(r/M) Plus@@Append[Table[Re[Exp[tS](1+I sigma) F[S] ],
{theta, Pi/M, (M-1)Pi/M, Pi/M}],
(1/2) Exp[rt] F[r] ]
```

When  $\bar{f}(s) = 1/(s^3 - 8)$  and we require the inverse transform for  $t = 0.5, 1, \dots, 2^6$  we need to implement the above with the instruction

```
Do[Print[FT[ $\frac{1}{\#^3-8}$  &, 2k, 300]], {k, -1, 6}]
```

### Mathematica program for Gaver's method

Abate and Valkó give a web reference for their GWR (Gaver Wynn rho) algorithm. The program below was written independently by my colleague Dr. R. Behrend.

```
F[f_ , n_ , t_ , M_]:=Module[ $\{np, a, np=Max[M, $MachinePrecision];$ 
 $a=SetPrecision[\frac{Log[2]}{t}, np];$ 
 $\frac{(2n)!}{n!(n-1)!}a \text{ Sum}[(-1)^k \text{ Binomial}[n, k] f[(k+n)a], \{k, 0, n\}]$ 
R[f_ , i_ , 0, t_ , M_]:=R[f, i, 0, t, M]=0;
R[f_ , i_ , 1, t_ , M_]:=R[f, i, 1, t, M]=F[f, i, t, M];
R[f_ , i_ , k_ , t_ , M_]:=R[f, i, k, t, M]
=R[f, i+1, k-2, t, M] +  $\frac{k-1}{R[f, i+1, k-1, t, M]-R[f, i, k-1, t, M]}$ 
```

Thus if we wanted to evaluate the inverse transform of  $1/(s^2 + 1)$  for  $t = 0.5, 1, \dots, 2^6$  we need to implement the above with the instruction

```
Do[Print[R[ $\frac{1}{\#^2+1}$  &, 1, 75, 2k, 300]], {k, -1, 6} ]
```

**Program for Application 1**  
**Gaver's method**

c Uses Gaver method in conjunction with the  $\rho$ -algorithm  
c Requires input of odd integer  $n \leq 45$   
c Requires input of variable  $t$   
c Requires a function subroutine `func(s,f)` to  
c evaluate the Laplace transform  $\bar{f}(s)$  for real  $s$ .

```
integer n
read(5,*)n
call gaver(n)
stop
end
```

```
subroutine gaver(n)
real rho1(45), rho2(45), a
m=n/2
if (n.eq.2*m) goto 100
do i=1, n
rho1(i)=0
enddo
call sequence (n, rho2)
do k=1, n-1
do i=1, n-k
rho1(i) =rho1(i+1)+ float(k)/(rho2(i+1)-rho2(i))
write(6,*)rho1(i)
enddo
write(6,*)'new cycle'
do i=1, n-k
a=rho1(i)
rho1(i)=rho2(i)
rho2(i)=a
enddo
enddo
goto 200
100 write(6,*)'Error, n not odd'
200 return
```

end

```
subroutine sequence(n, x)
real x(45), u(0:45,0:90), t, a, b, c, s, f, v, w
read(5,*)t
a=log(2.0)
a=a/t
m=2*n
do k=1, m
s=k*a
call funct(s, f)
u(0,k)=k*a*f
enddo
do k=1, n
do i=1, k
do j=k, 2*k-i
b=float(j)/float(i)
u(i, j)=(1+b)*u(i-1, j)-b*u(i-1, j+1)
enddo
enddo
x(k)=u(k, k)
write(6,*)x(k)
enddo
return
end
```

```
subroutine funct(s, f)
c Evaluation of this function requires the
c subroutine newton(s, z)
real s, f, z
f=1.0/s
call newton(s, z)
f=-f/(1.0-z)
return
end
```

```
subroutine newton(s, z)
real x, s, t, z, y0, y1
x=(s+4)/3
```

```
100  y0=x*x*x-((s+4)/3)*x*x+(1.0/3.0)
      y1=3*x*x-2*((s+4)/3)*x
      z=-y0/y1
      if (abs(z).lt.1.-16) goto 200
      x=x+z
      goto 100
200  z=x+z
      return
      end
```

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