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COULN, A PROGRAM FOR EVALUATING NEGATIVE ENERGY COULOMB FUNCTIONS

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PROGRAM SUMMARY

Title of program: COULN

Catalogue number: ACCU

Program obtainable from: CPC Program Library, Queen's University of Belfast, N. Ireland (see application form in this issue)

Computer: NAS 7000; *Installation:* SERC Daresbury Laboratory

Other machines on which the program has been tested: CRAY-1S, IBM 3081

Operating system: MVT

Programming language used: FORTRAN 77 (FORTRAN 66 compatible)

High speed storage required: 650 K (94 K for run step)

No. of bits in a byte: 8

Peripherals used: card reader, line printer

No. of lines in combined program and test deck: 450

Keywords: Coulomb, Whittaker, continued fraction, Padé, asymptotic, atomic, molecular, nuclear

Nature of the physical problem
Program COULN calculates exponentially decaying Whittaker functions, $W_{\kappa,\mu}(z)$ [1] corresponding to negative energy Coulomb functions. The method employed is most appropriate for parameter ranges which commonly occur in atomic and molecular asymptotic scattering problems using a close-coupling approximation in the presence of closed channels [2].

Method of solution
The asymptotic series for the Whittaker function is analytically continued using a continued fraction representation devised by Nesbet [3]. Functions corresponding to higher orbital angular momenta are computed by recursion.

Restrictions on the complexity of the problem
Program COULN assumes real negative energies, $E = -|k|^2$, non-negative real values of orbital angular momenta, l (integer), and separations, r. The charge product, Z, must be non-zero. The method becomes less efficient for large values of $|Z|$ and small values of the product $z = |k|r$. It is suitable for z/Z greater than 0.5 on IBM computers and greater than 0.1 on the CRAY-1S in double precision.

Typical running time
The test run required 5.2 s on the NAS 7000.

References
[1] M. Abramowitz and I.A. Stegun, eds., Handbook of Mathematical Functions (Dover, New York, 1965).
[2] C.J. Noble and R.K. Nesbet, Comput. Phys. Commun. 33 (1984) 399.
[3] R.K. Nesbet and C.J. Noble, (1984) to be published.

LONG WRITE-UP

1. Introduction

The exponentially decaying Whittaker function is a solution of the Coulomb differential equation corresponding to negative energies, $E = -k^2$, and therefore arises in a variety of different contexts in scattering problems involving charged particles. One important application occurs in the solution of the asymptotic problem which arises in atomic and molecular physics when using a close-coupling approximation in the presence of closed channels (see Noble and Nesbet, accompanying article [1]). Computer codes have therefore been written to evaluate these functions for both positive values of the charge product, Z [2] and also for negative values [3]. As in the case of the positive energy solutions [4] $E = k^2 > 0$, a number of different methods are necessary to cover the full parameter ranges which may occur in problems of physical interest. Thus, there are considerable difficulties in guaranteeing the accuracy of the values computed in all cases.

In the present work we describe a very simple computer code for evaluating the negative energy Coulomb functions and their first derivatives for both positive and negative Z values. Even though a single method is used, accurate results may be obtained over a very wide region of the parameter space including the region important in the solution of asymptotic scattering problems. In most situations the functions may be obtained with an accuracy within three or four digits of machine accuracy and in all cases an estimate of the error in the computed results is returned.

The Whittaker functions are calculated by analytically continuing their asymptotic expansion using a continued fraction algorithm devised by Nesbet [5]. Continued fractions are of course closely related to Padé approximants [6] and have been found to provide a useful and powerful tool when dealing with series in many branches of physics and mathematics. References to some of this work may be found in the book by Baker and Gammel [7]. The use of continued fraction expansions to analytically continue series expansions has also been emphasised by Hänggi et al. [8]. This particular property has not so far been used, as far as we are aware, in the calculation of Coulomb functions, although continued fraction expansions have been used to compute positive energy Coulomb functions [9]. The present code therefore provides a concrete example of these general methods for treating asymptotic series. A code capable of treating the entire real parameter range of physical interest could be constructed by adding a power series expansion of the functions about the origin incorporating, perhaps some of the suggestions of Frost and Harper [10]. A comprehensive code of this kind, allowing general complex parameter values and including such continuation techniques to provide both the irregular and regular solutions, has in fact been written [11] and will be published shortly. However, we believe that the simplicity of the present program will be valuable in a number of applications.

2. Theory

The required exponentially decaying Whittaker function is denoted by $W_{\kappa,\mu}(z)$ with $\kappa = 1/c = Z/\sqrt{-k^2}$, $\mu = l + 1/2$ and $z = \sqrt{-k^2}\, r$ in the notation of Abramowitz and Stegun [12]. It satisfies the differential equation

$$\frac{\mathrm{d}^2 W}{\mathrm{d}k^2} + \left[-c^2 + \frac{2}{x} - \frac{l(l+1)}{x^2} \right] W = 0, \tag{1}$$

where $x = Zr$. In these expressions r is the radial distance between the two particles with charge product Z, relative energy $E = -k^2 < 0$, and relative orbital angular momentum l. In program COULN the functions are evaluated by analytically continuing the asymptotic series (Abramowitz and Stegun [12], eq. 13.5.2)

$$\begin{aligned} &W_{1/c,l+1/2}(2cx) \\ &\quad \equiv V_l(c,x) \\ &\quad = \mathrm{e}^{-cx}(2cx)^{1/c} \sum_{n=0} \frac{(l+1-1/c)_n(-l-1/c)_n}{n!} \\ &\quad \times(-2cx)^{-n} \end{aligned} \tag{2}$$

by means of a continued fraction representation devised by Nesbet [5]. The Nth and $(N-1)$th convergents of the continued fraction are both evaluated in the form of a rational fraction allowing derivatives and error estimates to be calculated.

It should be noted that the asymptotic series (2) may terminate if $1/c$ is an integer greater than $1-L$ as a result of one of the numerator terms becoming zero. In these cases we evaluate the series (2) explicitly and bypass the analytical continuation.

Finally, as in the program of Bell and Scott [2], we obtain Whittaker functions for higher l values using the recursion relations

$$V_l = \left[\left(1 - \frac{l^2}{x}\right)V_{l-1} + lV'_{l-1}\right]/(1-cl), \quad (3)$$

$$V_l' = \left[\left(1 - \frac{l^2}{x}\right)V_l - (1+cl)V_{l-1}\right]/l, \quad (4)$$

where the prime denotes differentiation with respect to x. Upwards recursion on the parameter l using the relations (3) and (4) is stable only as long as $x < l^2$, as this condition determines the sign of the coefficient $(1 - l^2/x)$ multiplying the functions. For $x > 0$ it is important, therefore, that the recursion is started with function values computed from the accelerated asymptotic series at a value l_i chosen so that $l_i > \sqrt{x}$.

3. Code description

The program for evaluating the negative energy Whittaker functions and their derivatives consists of a main subroutine COULN and two utility routines, DFRACT and HSUM. Subroutine DFRACT is called by COULN to compute the coefficients of the continued fraction corresponding to a given number of terms of the asymptotic series (2). The algorithm used was devised by Nesbet [5]. The subroutine HSUM is called by COULN to evaluate the series (2) in the special terminating cases and uses Horner's algorithm.

The arguments of COULN are as follows:

L > 0	the orbital angular momentum value required, l;
Z real	the charge product;
E < 0	the energy (rydbergs);
R > 0	the radial separation (Bohr), r;
F	exponentially decaying Whittaker function value returned;
FP	derivative of Whittaker functions with respect to r;
ACC	accuracy required in function value;
EFX	estimated accuracy of value returned based on difference between nth and $(n-1)$th convergents;
XG XA XC XD	work arrays, these should be dimensioned in the calling routine to NTERM * KKKMAX + 1 according to the values of these parameters set by DATA statements in COULN;
IERR	= 0 on return if estimated accuracy is better than required accuracy, = 1 if required accuracy not obtained, = 2 if input arguments are not within the allowed ranges, = 3 terminating series case;
NLAST	the number of terms of the asymptotic series actually used. The terms are calculated NTERM at a time and the accuracy obtained is tested after each group. Up to KKKMAX groups may be tried so that NLAST < NTERM * KKKMAX.
FNORM	scale factor by which results F, FP should be multiplied.

The efficiency of the continuation method used by routine COULN decreases for larger values of the charge product, Z, and for smaller values of $z = |k|r$. Ultimately the accuracy which can be obtained in these cases is limited by round-off errors or by the permissible exponent range as increasingly large terms in the series (2) must be considered. We have verified the accuracy estimate EFX by comparison with the general program [11], and find our method is useful for values of the ratio z/Z greater than 0.5 on IBM computers, and greater than 0.1 on the CRAY-1S in double precision. For values outside these ranges, alternative methods [2,11] must use series expansions about the origin.

Finally, to improve efficiency, COULN should be adapted to return arrays of functions and derivatives if a range of l-values are required (keeping all other parameters constant) by saving the results of the recursion procedure.

4. Test deck

A small driver routine has been added to read input data, call subroutines COULN, DFRACT and HSUM and to print the results.

References

[1] C.J. Noble and R.K. Nesbet, Comput. Phys. Commun. 33 (1984) 399.

[2] K.L. Bell and N.S. Scott, Comput. Phys. Commun. 20 (1980) 447.

[3] D.F. Hebbard and B.A. Robson, Nucl. Phys. 42 (1963) 563.

[4] C. Bardin, Y. Dandeu, L. Gauthier, J. Guillermin, T. Lena, J.M. Pernet, H.H. Wolter and T. Tamura, Comput. Phys. Commun. 3 (1972) 73.

[5] R.K. Nesbet and C.J. Noble, to be published.

[6] H.S. Wall, Analytic Theory of Continued Fractions (Van Nostrand, New York, 1948).

[7] G.A. Baker and J.L. Gammel, eds., The Padé Approximant in Theoretical Physics (Academic Press, New York, 1970).

[8] P. Hänggi, F. Roesel and D. Trautmann, J. Comput. Phys. 37 (1980) 242.

[9] A.R. Barnett, Comput. Phys. Commun. 27 (1982) 147, and references therein.

[10] P.A. Frost and E.Y. Harper, SIAM Rev. 18 (1976) 62.

[11] I.J. Thompson and A.R. Barnett, (1984) to be published.

[12] M. Abramowitz and I.A. Stegun, eds., Handbook of Mathematical Functions (Dover, New York, 1965).

TEST RUN OUTPUT

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TEST RUN OUTPUT FOR EXPONENTIALLY DECAYING WHITTAKER FUNCTION ROUTINE COULN

ACC =  0.10000000D-11


      1 E = -0.10000000D+02 K =  0.31622777D+01 Z =   2 ETA = -0.63245553D+00 RHO =  0.20000000D+02 RATIO =  0.15811388D+02

L =  0 FX =  0.255306038902D-12 FXP = -0.791294380926D-12 FNORM =  0.100000000000D+01 EFX =.961D-16 IERR =  0 NLAST =    10
L =  1 FX =  0.263459341522D-12 FXP = -0.817387912238D-12 FNORM =  0.100000000000D+01 EFX =.112D-15 IERR =  0 NLAST =    10
L =  2 FX =  0.280546966837D-12 FXP = -0.872153358108D-12 FNORM =  0.100000000000D+01 EFX =.213D-14 IERR =  0 NLAST =    10
L =  3 FX =  0.308255629157D-12 FXP = -0.961171653059D-12 FNORM =  0.100000000000D+01 EFX =.111D-15 IERR =  0 NLAST =    20
L =  4 FX =  0.349454943811D-12 FXP = -0.109397220990D-11 FNORM =  0.100000000000D+01 EFX =.982D-16 IERR =  0 NLAST =    20
L =  5 FX =  0.408690885990D-12 FXP = -0.128572462817D-11 FNORM =  0.100000000000D+01 EFX =.982D-16 IERR =  0 NLAST =    20
L =  6 FX =  0.493013896104D-12 FXP = -0.156009472630D-11 FNORM =  0.100000000000D+01 EFX =.982D-16 IERR =  0 NLAST =    20
L =  7 FX =  0.613351110590D-12 FXP = -0.195401054594D-11 FNORM =  0.100000000000D+01 EFX =.982D-16 IERR =  0 NLAST =    20
L =  8 FX =  0.786790932781D-12 FXP = -0.252565930554D-11 FNORM =  0.100000000000D+01 EFX =.982D-16 IERR =  0 NLAST =    20
L =  9 FX =  0.104043232520D-11 FXP = -0.336807572877D-11 FNORM =  0.100000000000D+01 EFX =.982D-16 IERR =  0 NLAST =    20
L = 10 FX =  0.141797024817D-11 FXP = -0.463259856249D-11 FNORM =  0.100000000000D+01 EFX =.982D-16 IERR =  0 NLAST =    20
L = 11 FX =  0.199115374867D-11 FXP = -0.657006958019D-11 FNORM =  0.100000000000D+01 EFX =.982D-16 IERR =  0 NLAST =    20
L = 12 FX =  0.288007860139D-11 FXP = -0.960452119693D-11 FNORM =  0.100000000000D+01 EFX =.982D-16 IERR =  0 NLAST =    20
L = 13 FX =  0.428978832858D-11 FXP = -0.144674546283D-10 FNORM =  0.100000000000D+01 EFX =.982D-16 IERR =  0 NLAST =    20
L = 14 FX =  0.657753077796D-11 FXP = -0.224472245375D-10 FNORM =  0.100000000000D+01 EFX =.982D-16 IERR =  0 NLAST =    20
L = 15 FX =  0.103787040000D-10 FXP = -0.358612115420D-10 FNORM =  0.100000000000D+01 EFX =.982D-16 IERR =  0 NLAST =    20
L = 16 FX =  0.168472578629D-10 FXP = -0.589673871485D-10 FNORM =  0.100000000000D+01 EFX =.982D-16 IERR =  0 NLAST =    20
L = 17 FX =  0.281235086913D-10 FXP = -0.997590542055D-10 FNORM =  0.100000000000D+01 EFX =.982D-16 IERR =  0 NLAST =    20
L = 18 FX =  0.482623721724D-10 FXP = -0.173568961672D-09 FNORM =  0.100000000000D+01 EFX =.982D-16 IERR =  0 NLAST =    20
L = 19 FX =  0.851115422921D-10 FXP = -0.310452091690D-09 FNORM =  0.100000000000D+01 EFX =.982D-16 IERR =  0 NLAST =    20
L = 20 FX =  0.154187201307D-09 FXP = -0.570613165524D-09 FNORM =  0.100000000000D+01 EFX =.982D-16 IERR =  0 NLAST =    20


      2 E = -0.70100000D+01 K =  0.26476405D+01 Z =   2 ETA = -0.75538957D+00 RHO =  0.20000000D+02 RATIO =  0.13238202D+02

L =  0 FX =  0.638498544081D-10 FXP = -0.164250384794D-09 FNORM =  0.100000000000D+01 EFX =.206D-15 IERR =  0 NLAST =    10
L =  1 FX =  0.662955206447D-10 FXP = -0.170789677422D-09 FNORM =  0.100000000000D+01 EFX =.795D-15 IERR =  0 NLAST =    10
L =  2 FX =  0.714678134205D-10 FXP = -0.184647972616D-09 FNORM =  0.100000000000D+01 EFX =.774D-14 IERR =  0 NLAST =    10
L =  3 FX =  0.799824350581D-10 FXP = -0.207539390419D-09 FNORM =  0.100000000000D+01 EFX =.165D-15 IERR =  0 NLAST =    20
L =  4 FX =  0.929118028482D-10 FXP = -0.242464768311D-09 FNORM =  0.100000000000D+01 EFX =.000D+00 IERR =  0 NLAST =    20
L =  5 FX =  0.112008994851D-09 FXP = -0.294362668962D-09 FNORM =  0.100000000000D+01 EFX =.000D+00 IERR =  0 NLAST =    20
L =  6 FX =  0.140098835916D-09 FXP = -0.371255567731D-09 FNORM =  0.100000000000D+01 EFX =.000D+00 IERR =  0 NLAST =    20
L =  7 FX =  0.181756957055D-09 FXP = -0.486258895840D-09 FNORM =  0.100000000000D+01 EFX =.000D+00 IERR =  0 NLAST =    20
L =  8 FX =  0.244500888374D-09 FXP = -0.661141801067D-09 FNORM =  0.100000000000D+01 EFX =.000D+00 IERR =  0 NLAST =    20
L =  9 FX =  0.340914015292D-09 FXP = -0.932747918762D-09 FNORM =  0.100000000000D+01 EFX =.000D+00 IERR =  0 NLAST =    20
L = 10 FX =  0.492506620642D-09 FXP = -0.136480583949D-08 FNORM =  0.100000000000D+01 EFX =.000D+00 IERR =  0 NLAST =    20
L = 11 FX =  0.736880545176D-09 FXP = -0.207011743217D-08 FNORM =  0.100000000000D+01 EFX =.000D+00 IERR =  0 NLAST =    20
L = 12 FX =  0.114131018674D-08 FXP = -0.325316202866D-08 FNORM =  0.100000000000D+01 EFX =.000D+00 IERR =  0 NLAST =    20
L = 13 FX =  0.182905185061D-08 FXP = -0.529374002262D-08 FNORM =  0.100000000000D+01 EFX =.000D+00 IERR =  0 NLAST =    20
L = 14 FX =  0.303144764783D-08 FXP = -0.891492756003D-08 FNORM =  0.100000000000D+01 EFX =.000D+00 IERR =  0 NLAST =    20
L = 15 FX =  0.519344111899D-08 FXP = -0.155280793240D-07 FNORM =  0.100000000000D+01 EFX =.000D+00 IERR =  0 NLAST =    20
L = 16 FX =  0.919211649523D-08 FXP = -0.279579167983D-07 FNORM =  0.100000000000D+01 EFX =.000D+00 IERR =  0 NLAST =    20
L = 17 FX =  0.167996838915D-07 FXP = -0.520018742230D-07 FNORM =  0.100000000000D+01 EFX =.000D+00 IERR =  0 NLAST =    20
L = 18 FX =  0.316868692065D-07 FXP = -0.998617556392D-07 FNORM =  0.100000000000D+01 EFX =.000D+00 IERR =  0 NLAST =    20
L = 19 FX =  0.616475560683D-07 FXP = -0.197872036947D-06 FNORM =  0.100000000000D+01 EFX =.000D+00 IERR =  0 NLAST =    20
L = 20 FX =  0.123644760142D-06 FXP = -0.404310363519D-06 FNORM =  0.100000000000D+01 EFX =.000D+00 IERR =  0 NLAST =    20
```

```
      3 E = -0.40200000D+01 K =  0.20049938D+01 Z =   2 ETA = -0.99750934D+00 RHO =  0.20000000D+02 RATIO =  0.10024969D+02

L =  0 FX =  0.779111744788D-07 FXP = -0.148440189359D-06 FNORM =  0.100000000000D+01 EFX =.937D-16 IERR =  0 NLAST =    10
L =  1 FX =  0.818936819016D-07 FXP = -0.156435772444D-06 FNORM =  0.100000000000D+01 EFX =.000D+00 IERR =  0 NLAST =    10
L =  2 FX =  0.904690457160D-07 FXP = -0.173714766982D-06 FNORM =  0.100000000000D+01 EFX =.834D-15 IERR =  0 NLAST =    10
L =  3 FX =  0.105013777026D-06 FXP = -0.203197518206D-06 FNORM =  0.100000000000D+01 EFX =.282D-13 IERR =  0 NLAST =    10
L =  4 FX =  0.128037833054D-06 FXP = -0.250255073444D-06 FNORM =  0.100000000000D+01 EFX =.000D+00 IERR =  0 NLAST =    20
L =  5 FX =  0.163900235871D-06 FXP = -0.324320213839D-06 FNORM =  0.100000000000D+01 EFX =.000D+00 IERR =  0 NLAST =    20
L =  6 FX =  0.220156520012D-06 FXP = -0.441960768391D-06 FNORM =  0.100000000000D+01 EFX =.000D+00 IERR =  0 NLAST =    20
L =  7 FX =  0.310111576264D-06 FXP = -0.632789108817D-06 FNORM =  0.100000000000D+01 EFX =.000D+00 IERR =  0 NLAST =    20
L =  8 FX =  0.457751184944D-06 FXP = -0.951062822828D-06 FNORM =  0.100000000000D+01 EFX =.000D+00 IERR =  0 NLAST =    20
L =  9 FX =  0.707503105732D-06 FXP = -0.149904064032D-05 FNORM =  0.100000000000D+01 EFX =.000D+00 IERR =  0 NLAST =    20
L = 10 FX =  0.114407216484D-05 FXP = -0.247529766914D-05 FNORM =  0.100000000000D+01 EFX =.000D+00 IERR =  0 NLAST =    20
L = 11 FX =  0.193385868097D-05 FXP = -0.427750455854D-05 FNORM =  0.100000000000D+01 EFX =.000D+00 IERR =  0 NLAST =    20
L = 12 FX =  0.341387841112D-05 FXP = -0.772735873716D-05 FNORM =  0.100000000000D+01 EFX =.000D+00 IERR =  0 NLAST =    20
L = 13 FX =  0.628809314536D-05 FXP = -0.145771391375D-04 FNORM =  0.100000000000D+01 EFX =.000D+00 IERR =  0 NLAST =    20
L = 14 FX =  0.120733195652D-04 FXP = -0.286837740280D-04 FNORM =  0.100000000000D+01 EFX =.000D+00 IERR =  0 NLAST =    20
L = 15 FX =  0.241411191130D-04 FXP = -0.588095691879D-04 FNORM =  0.100000000000D+01 EFX =.000D+00 IERR =  0 NLAST =    20
L = 16 FX =  0.502223579718D-04 FXP = -0.125498411213D-03 FNORM =  0.100000000000D+01 EFX =.000D+00 IERR =  0 NLAST =    20
L = 17 FX =  0.108601088676D-03 FXP = -0.278449279410D-03 FNORM =  0.100000000000D+01 EFX =.000D+00 IERR =  0 NLAST =    20
L = 18 FX =  0.243871736355D-03 FXP = -0.641683559205D-03 FNORM =  0.100000000000D+01 EFX =.000D+00 IERR =  0 NLAST =    20
L = 19 FX =  0.568169584058D-03 FXP = -0.153434690515D-02 FNORM =  0.100000000000D+01 EFX =.000D+00 IERR =  0 NLAST =    20
L = 20 FX =  0.137211426205D-02 FXP = -0.380301053013D-02 FNORM =  0.100000000000D+01 EFX =.000D+00 IERR =  0 NLAST =    20
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```
TEST RUN OUTPUT FOR EXPONENTIALLY DECAYING WHITTAKER FUNCTION ROUTINE COULN

ACC =  0.10000000D-11


      1 E = -0.21000000D+00 K =  0.45825757D+00 Z =   2 ETA = -0.43643578D+01 RHO =  0.20000000D+01 RATIO =  0.22912878D+00

L =  0 FX = -0.670638380658D+01 FXP =  0.624018029228D+01 FNORM =  0.100000000000D+01 EFX =.921D-08 IERR =  1 NLAST =    70
L =  1 FX = -0.302387613094D+00 FXP =  0.161836307482D+02 FNORM =  0.100000000000D+01 EFX =.260D-05 IERR =  1 NLAST =    70
L =  2 FX =  0.304314697040D+02 FXP = -0.299905106783D+02 FNORM =  0.100000000000D+01 EFX =.260D-05 IERR =  1 NLAST =    70
L =  3 FX = -0.484610675311D+03 FXP =  0.109652514458D+04 FNORM =  0.100000000000D+01 EFX =.260D-05 IERR =  1 NLAST =    70
L =  4 FX =  0.669022496875D+05 FXP = -0.233693492058D+06 FNORM =  0.100000000000D+01 EFX =.260D-05 IERR =  1 NLAST =    70
L =  5 FX =  0.929396549339D+07 FXP = -0.428096606318D+08 FNORM =  0.100000000000D+01 EFX =.260D-05 IERR =  1 NLAST =    70
L =  6 FX =  0.764266951133D+09 FXP = -0.433820307496D+10 FNORM =  0.100000000000D+01 EFX =.260D-05 IERR =  1 NLAST =    70
L =  7 FX =  0.548830968052D+11 FXP = -0.369069385936D+12 FNORM =  0.100000000000D+01 EFX =.260D-05 IERR =  1 NLAST =    70
L =  8 FX =  0.381457148521D+13 FXP = -0.296018003791D+14 FNORM =  0.100000000000D+01 EFX =.260D-05 IERR =  1 NLAST =    70
L =  9 FX =  0.267270397940D+15 FXP = -0.234863589851D+16 FNORM =  0.100000000000D+01 EFX =.260D-05 IERR =  1 NLAST =    70
L = 10 FX =  0.192361672420D+17 FXP = -0.188690371734D+18 FNORM =  0.100000000000D+01 EFX =.260D-05 IERR =  1 NLAST =    70

      2 E = -0.11000000D+00 K =  0.33166248D+00 Z =   2 ETA = -0.60302269D+01 RHO =  0.20000000D+01 RATIO =  0.16583124D+00

L =  0 FX =  0.529022953090D+01 FXP =  0.199071397065D+03 FNORM =  0.100000000000D+01 EFX =.117D-05 IERR =  1 NLAST =    60
L =  1 FX =  0.122494178304D+03 FXP =  0.110159103675D+03 FNORM =  0.100000000000D+01 EFX =.397D-07 IERR =  1 NLAST =    60
L =  2 FX = -0.184563551236D+02 FXP = -0.144664546024D+03 FNORM =  0.100000000000D+01 EFX =.397D-07 IERR =  1 NLAST =    60
L =  3 FX = -0.303278947410D+03 FXP =  0.726076394533D+03 FNORM =  0.100000000000D+01 EFX =.397D-07 IERR =  1 NLAST =    60
L =  4 FX =  0.106188608471D+05 FXP = -0.369137872436D+05 FNORM =  0.100000000000D+01 EFX =.397D-07 IERR =  1 NLAST =    60
L =  5 FX = -0.125495549048D+07 FXP =  0.576502583416D+07 FNORM =  0.100000000000D+01 EFX =.397D-07 IERR =  1 NLAST =    60
L =  6 FX =  0.770650097811D+10 FXP = -0.436693376692D+11 FNORM =  0.100000000000D+01 EFX =.397D-07 IERR =  1 NLAST =    60
L =  7 FX =  0.207653403098D+13 FXP = -0.139472005941D+14 FNORM =  0.100000000000D+01 EFX =.397D-07 IERR =  1 NLAST =    60
L =  8 FX =  0.367859752593D+15 FXP = -0.285212092453D+16 FNORM =  0.100000000000D+01 EFX =.397D-07 IERR =  1 NLAST =    60
L =  9 FX =  0.555655867708D+17 FXP = -0.487946124655D+18 FNORM =  0.100000000000D+01 EFX =.397D-07 IERR =  1 NLAST =    60
L = 10 FX =  0.784193706949D+19 FXP = -0.768805254186D+20 FNORM =  0.100000000000D+01 EFX =.397D-07 IERR =  1 NLAST =    60
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TEST RUN OUTPUT FOR EXPONENTIALLY DECAYING WHITTAKER FUNCTION ROUTINE COULN

ACC =  0.10000000D-11


      1 E = -0.25397958D+01 K =  0.15936737D+01 Z =  22 ETA = -0.13804583D+02 RHO =  0.55000000D+02 RATIO =  0.18109928D+00

L =  0 FX = -0.708084809705D+10 FXP = -0.394311829517D+10 FNORM =  0.100000000000D+01 EFX =.122D-13 IERR =  0 NLAST =    40
L =  1 FX = -0.768827444673D+10 FXP =  0.996491336248D+09 FNORM =  0.100000000000D+01 EFX =.267D-13 IERR =  0 NLAST =    40
L =  2 FX = -0.823104636079D+10 FXP =  0.128669466685D+11 FNORM =  0.100000000000D+01 EFX =.377D-13 IERR =  0 NLAST =    30
L =  3 FX = -0.655383883733D+10 FXP =  0.332817303934D+11 FNORM =  0.100000000000D+01 EFX =.187D-12 IERR =  0 NLAST =    30
L =  4 FX =  0.197673166450D+10 FXP =  0.542000475585D+11 FNORM =  0.100000000000D+01 EFX =.428D-12 IERR =  0 NLAST =    30
L =  5 FX =  0.210040447344D+11 FXP =  0.385618228112D+11 FNORM =  0.100000000000D+01 EFX =.475D-13 IERR =  0 NLAST =    30
L =  6 FX =  0.314361633527D+11 FXP = -0.706692837234D+11 FNORM =  0.100000000000D+01 EFX =.262D-12 IERR =  0 NLAST =    30
L =  7 FX = -0.386598308273D+11 FXP = -0.162153155830D+12 FNORM =  0.100000000000D+01 EFX =.495D-15 IERR =  0 NLAST =    50
L =  8 FX = -0.125186315939D+12 FXP =  0.224259531830D+12 FNORM =  0.100000000000D+01 EFX =.495D-15 IERR =  0 NLAST =    50
L =  9 FX =  0.433629469111D+12 FXP =  0.443418930681D+10 FNORM =  0.100000000000D+01 EFX =.495D-15 IERR =  0 NLAST =    50
L = 10 FX = -0.128000192333D+13 FXP =  0.658954757927D+12 FNORM =  0.100000000000D+01 EFX =.495D-15 IERR =  0 NLAST =    50
L = 11 FX =  0.918217500344D+13 FXP = -0.174373107854D+14 FNORM =  0.100000000000D+01 EFX =.495D-15 IERR =  0 NLAST =    50
L = 12 FX = -0.186421714177D+15 FXP =  0.521583707253D+15 FNORM =  0.100000000000D+01 EFX =.495D-15 IERR =  0 NLAST =    50
L = 13 FX =  0.119177320158D+17 FXP = -0.411911586366D+17 FNORM =  0.100000000000D+01 EFX =.495D-15 IERR =  0 NLAST =    50
L = 14 FX =  0.400998677685D+19 FXP = -0.161922389986D+20 FNORM =  0.100000000000D+01 EFX =.495D-15 IERR =  0 NLAST =    50
L = 15 FX =  0.270621634790D+21 FXP = -0.123909000204D+22 FNORM =  0.100000000000D+01 EFX =.495D-15 IERR =  0 NLAST =    50
L = 16 FX =  0.118851235806D+23 FXP = -0.605261333169D+23 FNORM =  0.100000000000D+01 EFX =.495D-15 IERR =  0 NLAST =    50
L = 17 FX =  0.420503049276D+24 FXP = -0.234956207517D+25 FNORM =  0.100000000000D+01 EFX =.495D-15 IERR =  0 NLAST =    50
L = 18 FX =  0.130925205701D+26 FXP = -0.794482713323D+26 FNORM =  0.100000000000D+01 EFX =.495D-15 IERR =  0 NLAST =    50
L = 19 FX =  0.375859525520D+27 FXP = -0.245735159367D+28 FNORM =  0.100000000000D+01 EFX =.495D-15 IERR =  0 NLAST =    50
L = 20 FX =  0.102310139653D+29 FXP = -0.716064392721D+29 FNORM =  0.100000000000D+01 EFX =.495D-15 IERR =  0 NLAST =    50
L = 21 FX =  0.268890222014D+30 FXP = -0.200400644941D+31 FNORM =  0.100000000000D+01 EFX =.495D-15 IERR =  0 NLAST =    50
L = 22 FX =  0.690842514272D+31 FXP = -0.545831296050D+32 FNORM =  0.100000000000D+01 EFX =.495D-15 IERR =  0 NLAST =    50
L = 23 FX =  0.175048641995D+33 FXP = -0.146062750904D+34 FNORM =  0.100000000000D+01 EFX =.495D-15 IERR =  0 NLAST =    50
L = 24 FX =  0.440266224133D+34 FXP = -0.386692154643D+35 FNORM =  0.100000000000D+01 EFX =.495D-15 IERR =  0 NLAST =    50
L = 25 FX =  0.110444727410D+36 FXP = -0.101814666369D+37 FNORM =  0.100000000000D+01 EFX =.495D-15 IERR =  0 NLAST =    50
L = 26 FX =  0.277359676965D+37 FXP = -0.267679829162D+38 FNORM =  0.100000000000D+01 EFX =.495D-15 IERR =  0 NLAST =    50
L = 27 FX =  0.699264817901D+38 FXP = -0.704909045933D+39 FNORM =  0.100000000000D+01 EFX =.495D-15 IERR =  0 NLAST =    50
L = 28 FX =  0.177378147404D+40 FXP = -0.186390492946D+41 FNORM =  0.100000000000D+01 EFX =.495D-15 IERR =  0 NLAST =    50
L = 29 FX =  0.453495616234D+41 FXP = -0.495824255293D+42 FNORM =  0.100000000000D+01 EFX =.495D-15 IERR =  0 NLAST =    50
L = 30 FX =  0.117019113758D+43 FXP = -0.132896822313D+44 FNORM =  0.100000000000D+01 EFX =.495D-15 IERR =  0 NLAST =    50

TEST RUN OUTPUT FOR EXPONENTIALLY DECAYING WHITTAKER FUNCTION ROUTINE COULN

ACC =  0.10000000D-11


      1 E = -0.48000000D+01 K =  0.21908902D+01 Z =   2 ETA = -0.91287093D+00 RHO =  0.30000000D+01 RATIO =  0.16431677D+01

L =  0 FX =  0.211079253225D+00 FXP = -0.335654369111D+00 FNORM =  0.100000000000D+01 EFX =.175D-15 IERR =  0 NLAST =    30
L =  1 FX =  0.284013303384D+00 FXP = -0.505925575586D+00 FNORM =  0.100000000000D+01 EFX =.391D-15 IERR =  0 NLAST =    30
L =  2 FX =  0.504325807345D+00 FXP = -0.107436387741D+01 FNORM =  0.100000000000D+01 EFX =.322D-14 IERR =  0 NLAST =    30
L =  3 FX =  0.114602498558D+01 FXP = -0.296917300306D+01 FNORM =  0.100000000000D+01 EFX =.322D-14 IERR =  0 NLAST =    30
L =  4 FX =  0.322447137116D+01 FXP = -0.100701820746D+02 FNORM =  0.100000000000D+01 EFX =.322D-14 IERR =  0 NLAST =    30
L =  5 FX =  0.109044268055D+02 FXP = -0.403405700020D+02 FNORM =  0.100000000000D+01 EFX =.322D-14 IERR =  0 NLAST =    30
L =  6 FX =  0.432414578698D+02 FXP = -0.186077223276D+03 FNORM =  0.100000000000D+01 EFX =.322D-14 IERR =  0 NLAST =    30
L =  7 FX =  0.197103050880D+03 FXP = -0.970591069875D+03 FNORM =  0.100000000000D+01 EFX =.322D-14 IERR =  0 NLAST =    30
L =  8 FX =  0.101630249254D+04 FXP = -0.564731124828D+04 FNORM =  0.100000000000D+01 EFX =.322D-14 IERR =  0 NLAST =    30
L =  9 FX =  0.585130715771D+04 FXP = -0.362600046668D+05 FNORM =  0.100000000000D+01 EFX =.322D-14 IERR =  0 NLAST =    30
L = 10 FX =  0.372187559628D+05 FXP = -0.254671121676D+06 FNORM =  0.100000000000D+01 EFX =.322D-14 IERR =  0 NLAST =    30
L = 11 FX =  0.259244868461D+06 FXP = -0.194230286010D+07 FNORM =  0.100000000000D+01 EFX =.322D-14 IERR =  0 NLAST =    30
L = 12 FX =  0.196275470834D+07 FXP = -0.159860964096D+08 FNORM =  0.100000000000D+01 EFX =.322D-14 IERR =  0 NLAST =    30
L = 13 FX =  0.160500576963D+08 FXP = -0.141233402766D+09 FNORM =  0.100000000000D+01 EFX =.322D-14 IERR =  0 NLAST =    30
L = 14 FX =  0.140984575732D+09 FXP = -0.133317216647D+10 FNORM =  0.100000000000D+01 EFX =.322D-14 IERR =  0 NLAST =    30
L = 15 FX =  0.132400711968D+10 FXP = -0.133912165872D+11 FNORM =  0.100000000000D+01 EFX =.322D-14 IERR =  0 NLAST =    30
L = 16 FX =  0.132380984767D+11 FXP = -0.142617876595D+12 FNORM =  0.100000000000D+01 EFX =.322D-14 IERR =  0 NLAST =    30
L = 17 FX =  0.140404290257D+12 FXP = -0.160529111508D+13 FNORM =  0.100000000000D+01 EFX =.322D-14 IERR =  0 NLAST =    30
L = 18 FX =  0.157446629389D+13 FXP = -0.190418656919D+14 FNORM =  0.100000000000D+01 EFX =.322D-14 IERR =  0 NLAST =    30
L = 19 FX =  0.186128060185D+14 FXP = -0.237418182944D+15 FNORM =  0.100000000000D+01 EFX =.322D-14 IERR =  0 NLAST =    30
L = 20 FX =  0.231350093042D+15 FXP = -0.310417279338D+16 FNORM =  0.100000000000D+01 EFX =.322D-14 IERR =  0 NLAST =    30
L = 21 FX =  0.301626431642D+16 FXP = -0.424693331624D+17 FNORM =  0.100000000000D+01 EFX =.322D-14 IERR =  0 NLAST =    30
L = 22 FX =  0.411592604396D+17 FXP = -0.606809912034D+18 FNORM =  0.100000000000D+01 EFX =.322D-14 IERR =  0 NLAST =    30
L = 23 FX =  0.586681748157D+18 FXP = -0.903852548859D+19 FNORM =  0.100000000000D+01 EFX =.322D-14 IERR =  0 NLAST =    30
L = 24 FX =  0.871935810716D+19 FXP = -0.140117361995D+21 FNORM =  0.100000000000D+01 EFX =.322D-14 IERR =  0 NLAST =    30
L = 25 FX =  0.134892115381D+21 FXP = -0.225721125893D+22 FNORM =  0.100000000000D+01 EFX =.322D-14 IERR =  0 NLAST =    30
L = 26 FX =  0.216889128840D+22 FXP = -0.377331880084D+23 FNORM =  0.100000000000D+01 EFX =.322D-14 IERR =  0 NLAST =    30
L = 27 FX =  0.361923601019D+23 FXP = -0.653694027619D+24 FNORM =  0.100000000000D+01 EFX =.322D-14 IERR =  0 NLAST =    30
L = 28 FX =  0.625960642206D+24 FXP = -0.117217658368D+26 FNORM =  0.100000000000D+01 EFX =.322D-14 IERR =  0 NLAST =    30
L = 29 FX =  0.112070431827D+26 FXP = -0.217311182758D+27 FNORM =  0.100000000000D+01 EFX =.322D-14 IERR =  0 NLAST =    30
L = 30 FX =  0.207466350437D+27 FXP = -0.416079645633D+28 FNORM =  0.100000000000D+01 EFX =.322D-14 IERR =  0 NLAST =    30
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