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PROLATE ANGULAR SPHEROIDAL WAVE FUNCTIONS

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PROGRAM SUMMARY

Title of program: PASWFN

Catalog number: ACEZ

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

Computer: FELIX C-256; *Installation*: University Computer Centre, Cluj-Napoca, Romania

Operating system: SIRIS 2/3

Programming language used: FORTRAN IV

High speed storage required: 7 Kwords

Number of bits in a word: 32

Peripherals used: card reader, line printer

Number of cards in combined program and test deck: 494

Card punching code: EBCDIC

Keywords: general purpose, two centre frame, angular spheroidal wave functions, associated Legendre functions

Nature of the physical problem
The prolate angular spheroidal wave functions are required in problems concerning the angular aspects of the solution of the Schrödinger equation in a two centre frame. The package PASWFN contains six subprograms which compute these functions of the first kind (the functions of the second kind are of minor physical interest) for any argument and accuracy.

Method of solution
The prolate angular spheroidal wave functions $S_{ml}(c, \eta)$ are calculated as series of associated Legendre functions of the first kind. The coefficients are calculated separately, for given values of m, l, c [1], and are stored to be used in subsequent computations of $S_{ml}(c, \eta)$ for different values of η.

Typical running time
21 s for the test run.

Reference
[1] T.A. Beu and R.I. Câmpeanu, Comput. Phys. Commun. 30 (1983) 177.

LONG WRITE-UP

1. Introduction

The prolate angular spheroidal wave function is the angular component of the solution of the Schrödinger equation for the field-free space $(\nabla^2 + k^2)\psi = 0$ in a two-centre frame. This function satisfies the angular equation:

$$\frac{\mathrm{d}}{\mathrm{d}\eta}\left[(1-\eta^2)\frac{\mathrm{d}}{\mathrm{d}\eta}S_{ml}(c,\eta)\right] + \left[\lambda_{ml} - c^2\eta^2 - \frac{m^2}{1-\eta^2}\right]S_{ml}(c,\eta) = 0, \tag{1}$$

where $c = kd/2$, d being the distance between the two centres, ξ and η the elliptical coordinates and λ_{ml} are the separation constants (or eigenvalues), determined so that $S_{ml}(c, \eta)$ are finite at $\eta = \pm 1$. In this paper we are concerned with the calculation of $S^1_{ml}(c, \eta)$ for real η and k.

2. The calculation of $S^1_{ml}(c, \eta)$

The functions $S^1_{ml}(c, \eta)$ can be expressed as an associated Legendre function series:

$$S^1_{ml}(c,\eta) = \sum_{r=0,1}^{\infty}{}' \, d_r^{ml}(c) P^m_{m+r}(\eta), \tag{2}$$

where $P^m_n(\eta)$ are the associated Legendre functions of the first kind and $d_r^{ml}(c)$ are the coefficients of the expansion. The summation in (2) is extended over even or odd values of r, depending on whether $l - m$ is even or odd. The convergence of the series (2) is very good and so only a few terms have to be computed.

The procedure for calculating the coefficients $d_r^{ml}(c)$ has been described in a previous paper [1] and in this paper we shall concentrate on the computation of the functions $P^m_n(\eta)$.

3. Code description

The package consists of 6 suprograms: VALPROP, COEF, NORM, FFACT, S1 and P. The first 4 subroutines compute the coefficients $d_r^{ml}(c)$ and were discussed in ref. [1]. The subroutine P evaluates the associated Legendre functions of the first kind, which, together with the coefficients $d_r^{ml}(c)$, are the input for the function type subprogram S1, which actually calculates the prolate angular spheroidal functions.

As in ref. [1], the main program has to call first the subroutines VALPROP, COEF, NORM and only after this can it employ the prolate angular spheroidal functions given by FUNCTION S1.

As an example we give the following sequence of instructions:

```
DIMENSION D(10), ORD(10)
NIT = 10
...
CALL VALPROP
CALL COEF(NIT, D, ORD)
CALL NORM(NIT, D, ORD)
...
S = S1(ETA, NIT, D, ORD)
...
STOP
END
```

The variable ETA contains the value of the angle given in radians.

FUNCTION P uses the following expression in calculating the associated Legendre functions of the first kind:

$$P_n^m(x) = \left[-\tfrac{1}{2}\sqrt{1-x^2}\right]^m \frac{(-n)_m (n+1)_m}{m!} \sum_{k=0}^{n-m} \frac{(-n+m)_k (n+m+1)_k}{(m+1)_k k!} \left[\frac{1-x}{2}\right]^k, \tag{3}$$

where m, n are integers and $(n)_m$ is Pochhammer's symbol: $(n)_m = n(n+1)\dots(n+m-1)$. The proof of expression (3) is presented in the appendix.

FUNCTION S1 calculates the prolate angular spheroidal functions by employing the expansion (2), with the coefficients $d_r^{ml}(c)$ provided by VALPROP, COEF and NORM. The functions $P_n^m(x)$ are calculated with the recurrence relation:

$$(n-m+1)P_{n+1}^m(x) = (2n+1)xP_n^m(x) - (n+m)P_{n-1}^m(x), \tag{4}$$

where the first two functions are given by FUNCTION P.

The subprogram terminates when the relative accuracy ERRB is achieved, i.e. when the absolute value of the ratio of the last added term to the value of the calculated sum is less than or equal to ERRB. The number of terms in (2) corresponding to ERRB is stored in the variable NT1 and can be printed in the main program.

The COMMON block SF is the same as in ref. [1].

The input in the main program consists of values for the following variables: ERRB, ERRV, ERRD, NIT, L, M, C, ETA. The output in the main program can include, as well as the values of $S_{ml}^1(c, \eta)$, the values of NT1, of the eigenvalue VAL and of the coefficients (D and ORD).

4. Test deck and accuracy checks

The test deck contains a main program which calls the subprograms of PASWFN for $l = 0(1)3$, $m = 0(1)l$, $c = 1.(1.)5.$, $\eta = 0°(10°)90°$ and lists the results in a tabular form employed by ref. [2]. The program is in single precision, with ERRV, ERRB, ERRD set to 10^{-6}. This precision is sufficient to obtain excellent agreement with the results tabulated in ref. [2], and was achieved by taking in the expansion (2) a maximum number of 10 terms (this can be easily checked by listing the values of NT1). Therefore, in this test run we used NIT = 10.

If for some application one wishes to run the subroutines in double precision, one has to give appropriate values to the error variables and include the cards:

```
ABS(X) = DABS(X)         ...  VALPROP, COEF, S1
SQRT(X) = DSQRT(X)       ...  P
INT(X) = IDINT(X)        ...  VALPROP, NORM
FLOAT(I) = DFLOAT(I)     ...  FFACT
```

at the beginning of the subprograms mentioned on the right hand side.

Appendix

The associated Legendre functions are given by:

$$P_n^m(x) = (1-x^2)^{\frac{1}{2}m} \mathrm{d}^m P_n(x)/\mathrm{d}x^m,$$

where the Legendre polynomials can be expressed as hypergeometric functions:

$$P_n(x) = (-1)^m F(-n, n+1;\ 1;\ (1-x)/2)$$

with

$$F(a, b;\ c;\ x) = \sum_{k=0}^{\infty} \frac{(a)_k (b)_k}{(c)_k} \frac{x^k}{k!}.$$

On the other hand

$$\frac{\mathrm{d}^m}{\mathrm{d}x^m} F(a, b;\ c;\ x) = \frac{(a)_m (b)_m}{(c)_m} F(a+m, b+m;\ c+m;\ x)$$

and therefore:

$$P_n^m(x) = \left[-\tfrac{1}{2}(1-x^2)^{1/2}\right]^m \frac{(-n)_m (n+1)_m}{m!} F\left(-n+m, n+m+1;\ m+1;\ \frac{1-x}{2}\right).$$

From this result one obtains eq. (3) if one takes into account that $(-n)_k = 0$ for $k > n$.

References

[1] T.A. Beu and R.I. Câmpeanu, Comput. Phys. Commun. 30 (1983) 177.

[2] Handbook of Mathematical Functions with Formulas, Graphs and Mathematical Tables, eds. M. Abramowitz and I.A. Stegun (Dover, New York, 1970).

TEST RUN OUTPUT

```
   NIT=   10
ERRR= 1.0E-06
```

M	L	C	0(DEG)	10(DEG)	20(DEG)	30(DEG)	40(DEG)	50(DEG)	60(DEG)	70(DEG)	80(DEG)	90(DEG)
0	0	1.	8.4814E-01	8.5250E-01	8.6513E-01	8.8470E-01	9.0906E-01	9.3542E-01	9.6061E-01	9.8145E-01	9.9520E-01	1.0000E+00
0	0	2.	5.3151E-01	5.4309E-01	5.7724E-01	6.3196E-01	7.0319E-01	7.8419E-01	8.6541E-01	9.3545E-01	9.8309E-01	1.0000E+00
0	0	3.	2.6749E-01	2.8153E-01	3.2425E-01	3.9667E-01	4.9802E-01	6.2260E-01	7.5709E-01	8.8046E-01	9.6815E-01	1.0000E+00
0	0	4.	1.1935E-01	1.3119E-01	1.6887E-01	2.3790E-01	3.4423E-01	4.8848E-01	6.5889E-01	8.2712E-01	9.5304E-01	1.0000E+00
0	0	5.	5.0230E-02	5.8440E-02	8.6083E-02	1.4186E-01	2.3803E-01	3.8393E-01	5.7422E-01	7.7756E-01	9.3834E-01	1.0000E+00
0	1	1.	9.0460E-01	8.9359E-01	8.6020E-01	8.0351E-01	7.2253E-01	6.1692E-01	4.8775E-01	3.3808E-01	1.7313E-01	.0000E+00
0	1	2.	6.6812E-01	6.6650E-01	6.5983E-01	6.4289E-01	6.0809E-01	5.4719E-01	4.5398E-01	3.2702E-01	1.7166E-01	.0000E+00
0	1	3.	4.0339E-01	4.0991E-01	4.2731E-01	4.4888E-01	4.6303E-01	4.5426E-01	4.0683E-01	3.1099E-01	1.6948E-01	.0000E+00
0	1	4.	2.0419E-01	2.1376E-01	2.4148E-01	2.8333E-01	3.2941E-01	3.6180E-01	3.5657E-01	2.9295E-01	1.6694E-01	.0000E+00
0	1	5.	9.1606E-02	1.0011E-01	1.2623E-01	1.7031E-01	2.2795E-01	2.8399E-01	3.1037E-01	2.7521E-01	1.6433E-01	.0000E+00
0	2	1.	1.0222E+00	9.7945E-01	8.5533E-01	6.6206E-01	4.1978E-01	1.5558E-01	-9.8751E-02	-3.1049E-01	-4.5085E-01	-5.0000E-01
0	2	2.	1.0640E+00	1.0298E+00	9.2713E-01	7.5787E-01	5.2955E-01	2.6017E-01	-1.9238E-02	-2.6685E-01	-4.3849E-01	-5.0000E-01
0	2	3.	1.0409E+00	1.0231E+00	9.6396E-01	8.4971E-01	6.6594E-01	4.1041E-01	1.0609E-01	-1.9378E-01	-4.1705E-01	-5.0000E-01
0	2	4.	8.7288E-01	8.7670E-01	8.7863E-01	8.5118E-01	7.5487E-01	5.5524E-01	2.5124E-01	-9.9809E-02	-3.8788E-01	-5.0000E-01
0	2	5.	6.0174E-01	6.2318E-01	6.7908E-01	7.4056E-01	7.5362E-01	6.4927E-01	3.8439E-01	7.9266E-04	-3.5415E-01	-5.0000E-01
0	3	1.	9.8917E-01	9.0415E-01	6.6917E-01	3.3999E-01	-4.5426E-03	-2.8157E-01	-4.2585E-01	-4.0853E-01	-2.4673E-01	.0000E+00
0	3	2.	9.5902E-01	8.8636E-01	6.8159E-01	3.8400E-01	5.6018E-02	-2.2614E-01	-3.9075E-01	-3.9486E-01	-2.4473E-01	.0000E+00
0	3	3.	9.0896E-01	8.5464E-01	6.9575E-01	4.4850E-01	1.5008E-01	-1.3640E-01	-3.3194E-01	-3.7136E-01	-2.4123E-01	.0000E+00
0	3	4.	8.1971E-01	7.8771E-01	6.8682E-01	5.0870E-01	2.5906E-01	-2.1449E-02	-2.5137E-01	-3.3761E-01	-2.3606E-01	.0000E+00
0	3	5.	6.6497E-01	6.5599E-01	6.1831E-01	5.2450E-01	3.4823E-01	9.7087E-02	-1.5751E-01	-2.9520E-01	-2.2928E-01	.0000E+00
1	1	1.	.0000E+00	1.5773E-01	3.1339E-01	4.6429E-01	6.0665E-01	7.3554E-01	8.4504E-01	9.2899E-01	9.8191E-01	1.0000E+00
1	1	2.	.0000E+00	1.1944E-01	2.4366E-01	3.7566E-01	5.1493E-01	6.5620E-01	7.8921E-01	8.9998E-01	9.7395E-01	1.0000E+00
1	1	3.	.0000E+00	7.7562E-02	1.6545E-01	2.7235E-01	4.0295E-01	5.5457E-01	7.1444E-01	8.5973E-01	9.6266E-01	1.0000E+00
1	1	4.	.0000E+00	4.4854E-02	1.0186E-01	1.8324E-01	2.9938E-01	4.5368E-01	6.3534E-01	8.1496E-01	9.4969E-01	1.0000E+00
1	1	5.	.0000E+00	2.3929E-02	5.8836E-02	1.1790E-01	2.1619E-01	3.6504E-01	5.6016E-01	7.6975E-01	9.3608E-01	1.0000E+00
1	2	1.	.0000E+00	4.7874E-01	9.0536E-01	1.2315E+00	1.4168E+00	1.4345E+00	1.2762E+00	9.5623E-01	5.1194E-01	.0000E+00
1	2	2.	.0000E+00	3.8957E-01	7.5094E-01	1.0515E+00	1.2531E+00	1.3164E+00	1.2120E+00	9.3350E-01	5.0878E-01	.0000E+00
1	2	3.	.0000E+00	2.7797E-01	5.5383E-01	8.1478E-01	1.0297E+00	1.1491E+00	1.1176E+00	8.9916E-01	5.0393E-01	.0000E+00
1	2	4.	.0000E+00	1.7612E-01	3.6825E-01	5.8128E-01	7.9675E-01	9.6425E-01	1.0078E+00	8.5751E-01	4.9788E-01	.0000E+00
1	2	5.	.0000E+00	1.0109E-01	2.2543E-01	3.8960E-01	5.9064E-01	7.8788E-01	8.9573E-01	8.1267E-01	4.9115E-01	.0000E+00

1	3	1.	.0000E+00	9.9282E-01	1.7453E+00	2.0749E+00	1.9030E+00	1.2800E+00	3.7754E-01	-5.5206E-01	-1.2445E+00	-1.5000E+00
1	3	2.	.0000E+00	9.5586E-01	1.7103E+00	2.0924E+00	1.9985E+00	1.4322E+00	5.2985E-01	-4.5414E-01	-1.2143E+00	-1.5000E+00
1	3	3.	.0000E+00	8.7446E-01	1.6107E+00	2.0632E+00	2.0965E+00	1.6399E+00	7.6055E-01	-2.9722E-01	-1.1645E+00	-1.5000E+00
1	3	4.	.0000E+00	7.3922E-01	1.4182E+00	1.9336E+00	2.1276E+00	1.8405E+00	1.0318E+00	-9.5120E-02	-1.0972E+00	-1.5000E+00
1	3	5.	.0000E+00	5.6624E-01	1.1459E+00	1.6909E+00	2.0471E+00	1.9755E+00	1.2987E+00	1.3192E-01	-1.0168E+00	-1.5000E+00
2	2	1.	.0000E+00	8.4440E-02	3.2962E-01	7.1117E-01	1.1891E+00	1.7098E+00	2.2106E+00	2.6273E+00	2.9034E+00	3.0000E+00
2	2	2.	.0000E+00	6.9005E-02	2.7445E-01	6.0919E-01	1.0542E+00	1.5717E+00	2.1015E+00	2.5461E+00	2.8858E+00	3.0000E+00
2	2	3.	.0000E+00	5.0025E-02	2.0528E-01	4.7752E-01	8.7383E-01	1.3799E+00	1.9445E+00	2.4755E+00	2.8594E+00	3.0000E+00
2	2	4.	.0000E+00	3.2776E-02	1.4053E-01	3.4863E-01	6.8754E-01	1.1707E+00	1.7643E+00	2.3673E+00	2.8270E+00	3.0000E+00
2	2	5.	.0000E+00	1.9800E-02	8.9794E-02	2.4139E-01	5.2128E-01	9.7015E-01	1.5802E+00	2.2511E+00	2.7911E+00	3.0000E+00
2	3	1.	.0000E+00	4.2211E-01	1.5701E+00	3.1154E+00	4.5959E+00	5.5302E+00	5.5478E+00	4.5010E+00	2.5220E+00	.0000E+00
2	3	2.	.0000E+00	3.5966E-01	1.3576E+00	2.7545E+00	4.1755E+00	5.1705E+00	5.3274E+00	4.4167E+00	2.5097E+00	.0000E+00
2	3	3.	.0000E+00	2.7665E-01	1.0705E+00	2.2552E+00	3.5763E+00	4.6415E+00	4.9939E+00	4.2861E+00	2.4905E+00	.0000E+00
2	3	4.	.0000E+00	1.9352E-01	7.7592E-01	1.7233E+00	2.9091E+00	4.0247E+00	4.5878E+00	4.1215E+00	2.4657E+00	.0000E+00
2	3	5.	.0000E+00	1.2441E-01	5.2265E-01	1.2426E+00	2.2690E+00	3.3955E+00	4.1499E+00	3.9361E+00	2.4370E+00	.0000E+00