8. Conclusion

Because the output of one pass is read backwards by the next pass, this method is particularly suited to machines with tapes that can be read in either direction. Disk files or drums are also suitable for the intermediate storage, and can lead to very fast second and third passes.

On a machine with a large main memory many methods of optimization which use large parts of core are feasible. Since the first pass is usually highly input limited, it might be an advantage to use the method outlined above on several programs simultaneously; that is, the compiler program is time-shared by several inputs and auxiliary devices, each using a small piece of memory for data storage.

Partial optimization of the object code in a machine independent fashion is certainly feasible using a small amount of main memory with a reversible auxiliary store. On most machines it is likely that the input time for the source program will dominate the compile speed. Optimization of the use of machine features such as index registers is a harder problem, probably requiring two further passes, one in each direction, since in the proposed compiler, information about which addresses would best be in index registers is not available until pass II, and pass II must generate code whose length can be determined by the end of pass II.

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Draft Specification of COBOL Available

COBOL Information Bulletin \$6 contains a draft specification of COBOL produced by ASA Working Group X3.4.4. The specification is a working document in the standardization process. ASA Subcommittee X3.4 has authorized publication of the specification to elicit comment and criticism. The document, with whatever changes it may undergo during evaluation, is intended to be the basis for a standard to be adopted by the American Standards Association.

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J. G. HERRIOT, Editor

ALGORITHM 259

LEGENDRE FUNCTIONS FOR ARGUMENTS LARGER THAN ONE* [S16]

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*Work performed in part under the auspices of the U.S. Atomic Energy Commission.

begin

comment Control is transferred to a nonlocal label, called *alarm*, whenever the input variables are not in the intended range;

procedure integer Legendre 1 (x, a, nmax, P);

value x, a, nmax; integer a, nmax; real x; array P; comment This procedure generates the associated Legendre functions of the first kind,

$$P_a{}^n(x) = \frac{(x^2-1)^{n/2}}{2^a a!} \frac{d^{a+n}}{dx^{a+n}} (x^2-1)^a,$$

for n = 0(1)nmax, assuming $a \ge 0$ an integer, and x > 1. The results are stored in the array P. The method of computation is derived from the (finite) continued fraction

$$(n+a)F_n/F_{n-1} = \frac{(n+a)(a+1-n)}{nx_1+} \frac{(n+a+1)(a-n)}{(n+1)x_1+}$$

$$\frac{(n+a+2) (a-n-1)}{(n+2)x_1+} \cdots \frac{2a \cdot 1}{ax_1} \quad (1 \le n \le a),$$

where $F_n = P_a^n(x)/(n+a)!$, $x_1 = 2x(x^2-1)^{-\frac{1}{2}}$, and the identity

$$F_0 + 2 \sum_{n=1}^{a} F_n = [x + (x^2 - 1)^{\frac{1}{2}}]^a / a!$$

If x is very close to 1, the computation of x_1 is subject to cancellation of significant digits. In such cases it would be better to use y = x-1 as input variable, and to compute $(x^2-1)^{\frac{1}{2}}$ by $[y(2+y)]^{\frac{1}{2}}$ everywhere in the procedure body;

begin integer n; real x1, c, sum, r, s;

array Rr[0:nmax-1];

if $x < 1 \lor a < 0 \lor nmax < 0$ then go to alarm;

if $x = 1 \lor a = 0$ then

begin

P[0] := 1; for n := 1 step 1 until nmax do $P[n]_{\frac{1}{4}}^{\frac{3}{4}} := 0$; go to L

end;

for n := a+1 step 1 until nmax do P[n] := 0;

 $x1 := sqrt (x \uparrow 2-1);$

c := 1; for n := 2 step 1 until a do $c := n \times c$;

 $sum := (x+x1) \uparrow a/c; x1 := 2 \times x/x1;$

r := s := 0;

for n := a step - 1 until 1 do

begin

 $r := (a+1-n)/(n \times x1 + (n+a+1) \times r); \quad s := r \times (2+s);$ if $n \le nmax$ then Rr[n-1] := r

end;

 $P[0] := c \times sum/(1+s);$

for n := 0 step 1 until if $nmax \le a$ then nmax-1 else a-1 do $P[n+1] := (n+a+1) \times Rr[n] \times P[n];$

L: end integer Legendre 1;

procedure integer Legendre 2(x, m, nmax, d, Q);

value x, m, nmax, d; integer m, nmax, d; real x; array Q; comment This procedure generates to d significant digits the associated Legendre functions of the second kind, $Q_n^m(x)$, for n = O(1)nmax, assuming $m \ge 0$ an integer, and x > 1. The results are stored in the array Q. The procedure first generates $Q_0^m(x)$ from the recurrence relation

$$Q_n^{r+1} + \frac{2rx}{(x^2 - 1)^{\frac{1}{2}}} Q_n^r + (r + n)(r - n - 1)Q_n^{r-1} = 0$$

$$(r = 1, 2, \dots, m - 1)$$
(1)

with n = 0, and the initial values

$$Q_0{}^0(x) = rac{1}{2} \ln rac{x+1}{x-1}$$
, $Q_0{}^1(x) = -(x^2-1)^{-rac{1}{2}}$.

Then a variant of the backward recurrence algorithm of J. C. P. Miller is applied to the recursion

$$(n-m+1)Q_{n+1}^m - (2n+1)xQ_n^m + (n+m)Q_{n-1}^m = 0$$

$$(n=1, 2, 3, \cdots).$$
(2)

(For more details see [2]. See also [4] for a very similar algorithm.) If m>1, the leading coefficient in (2) vanishes for n=m-1, which invalidates the theoretical justification for the backward recurrence procedure. Nevertheless, it appears that the procedure produces valid results for arbitrary $m\geq 0$. Convergence of the backward recurrence algorithm is slow for x near 1, but improves rapidly as x increases;

```
begin integer n, nu, p; real x1, Q0, Q1, Q2, epsilon, r;
  array Qapprox, Rr[0: nmax];
  if x \le 1 \lor nmax < 0 \lor m < 0 then go to alarm;
 x1 := sqrt (x \uparrow 2 - 1);
 O1 := .5 \times ln ((x+1)/(x-1));
  if m = 0 then Q[0] := Q1 else
   Q2 := -1/x1; x1 := 2 \times x/x1;
    for n := 1 step 1 until m - 1 do
    begin
      Q0 := Q1; \quad Q1 := Q2;
        Q2 := -n \times x1 \times Q1 - n \times (n-1) \times Q0
    end;
   Q[0] := Q2
  end;
  for n := 0 step 1 until nmax do Qapprox[n] := 0;
  epsilon := .5 \times 10 \uparrow (-d);
  nu := 20 + entier (1.25 \times nmax);
L0: r := 0;
 for n := nu step -1 until 1 do
 begin
    r := (n+m)/((2\times n+1)\times x - (n-m+1)\times r);
   if n \leq nmax then Rr[n-1] := r
  for n := 0 step 1 until nmax-1 do Q[n+1] := Rr[n] \times Q[n];
  for n := 0 step 1 until nmax do
 if abs(Q[n]-Qapprox[n]) > epsilon \times abs(Q[n]) then
    for p := 0 step 1 until nmax do Qapprox[p] := Q[p];
   nu := nu + 10; go to L0
  end
end integer Legendre 2;
procedure integer Legendre 3(x, n, mmax, d, Q);
 value x, n, mmax, d; integer n, mmax, d; real x; array Q;
comment This procedure generates to d significant digits, and
```

stores in the array Q, the Legendre functions of the second kind,

 $Q_n^m(x)$, for m=0(1)mmax, assuming $n\geq 0$ an integer, and

x > 1. The procedure integer Legendre 2 is used to obtain initial values Q_n^0 , Q_n^1 , and subsequent values are obtained from the recursion (1) of the preceding comment;

begin integer m; real x1; array Q1[0:n]; if $n < 0 \lor mmax < 0$ then go to alarm; integer Legendre 2(x, 0, n, d, Q1); Q[0] := Q1[n]; $x1 := 2 \times x/sqrt(x\uparrow 2-1)$; if mmax > 0 then

begin

integer Legendre 2(x, 1, n, d, Q1); Q[1] := Q1[n] end;

for m := 1 step 1 until mmax-1 do

 $Q[m+1] := -m \times x1 \times Q[m] - (m+n) \times (m-n-1) \times Q[m-1]$ end integer Legendre 3;

procedure Legendre 1(x, alpha, nmax, d, P1);

value x, alpha, nmax, d; integer nmax, d;

real x, alpha; array P1;

 ${f comment}$ This procedure evaluates to d significant digits the Legendre functions

$$P_{\alpha}{}^n(x) = \frac{\Gamma(\alpha+n+1)}{\pi\Gamma(\alpha+1)} \int_0^{\pi} \left[x + (x^2-1)^{\frac{1}{2}}\cos t\right]^{\alpha} \cos nt \, dt$$

for n=0(1)nmax, where x>1 and α is real. The results are stored in the array P1. It is assumed that a nonlocal procedure gamma be available which evaluates $\Gamma(z)$ for $0< z \le 2$. (See [3].) The procedure first generates the quantities $f_n=P_{\alpha}{}^n(x)/\Gamma(\alpha+n+1)$ from the recurrence relation

$$f_{n+1} + \frac{2nx}{(n+\alpha+1)(x^2-1)^{\frac{1}{2}}}f_n + \frac{n-\alpha-1}{n+\alpha+1}f_{n-1} = 0,$$

and the identity

$$f_0 + 2 \sum_{n=1}^{\infty} f_n = \frac{[x + (x^2 - 1)^{\frac{1}{2}}]^{\alpha}}{\Gamma(\alpha + 1)},$$

applying a variant of the backward recurrence algorithm of J. C. P. Miller. (See [2] for more details.) Then $P_{\alpha}^{n}(x) = \Gamma(\alpha+n+1)f_{n}$ is obtained recursively. If $\alpha < -\frac{1}{2}$, we let $\alpha = -\alpha - 1$ and compute $P_{\alpha}^{n}(x) = P_{\alpha}^{n}(x)$. The substitution is made to avoid loss of accuracy when x is large. The rate of convergence of this procedure decreases as x increases. A general idea of the speed of convergence may be obtained from the graphs in [2, §6]. If x is very close to 1, the same changes as mentioned in the first procedure are recommended;

begin integer n, nu, m; real a, epsilon, x1, sum, c, r, s; array Papprox, Rr[0:nmax];

if $x < 1 \lor nmax < 0 \lor entier(alpha) - alpha = 0$ then

go to alarm; if x = 1 then

begin

P1[0] := 1; for n := 1 step 1 until nmax do P1[n] := 0; go to L1

end;

 $a := if \ alpha < -.5 \ then - alpha - 1 \ else \ alpha;$ for $n := 0 \ step \ 1 \ until \ nmax \ do \ Papprox[n] := 0;$

 $epsilon := .5 \times 10 \uparrow (-d);$

if $a \le 1$ then c := gamma(1+a) else

begin

 $m := entier(a) - 1; \quad c := gamma(a-m);$

for n := 0 step 1 until m do $c := (a-n) \times c$ and:

 $x1 := sqrt \ (x\uparrow 2-1); \quad sum := (x+x1)\uparrow a/c; \quad x1 := 2 \times x/x1;$ $nu := 20 + entier \ ((37.26+.1283\times(a+38.26)\times x)\times nmax/$ $(37.26+.1283\times(a+1)\times x));$

L0: r := s := 0;

for n := nu step -1 until 1 do

begin

 $r := (a+1-n)/(n \times x1 + (n+a+1) \times r); \quad s := r \times (2+s);$ if $n \le n \max$ then Rr[n-1] := r end;

```
P1[0] := sum/(1+s);
  for n := 0 step 1 until nmax - 1 do
    P1[n+1] := Rr[n] \times P1[n];
  for n := 0 step 1 until nmax do
    if abs\ (P1[n]-Papprox[n]) > epsilon \times abs\ (P1[n]) then
      for m := 0 step 1 until nmax do Papprox [m] := P1[m];
      nu := nu + 10; go to L0
  P1[0] := c \times P1[0];
  for n := 1 step 1 until nmax do
    c := (a+n) \times c; P1[n] := c \times P1[n]
  end;
L1: end Legendre 1;
procedure Legendre 2(x, a, m, nmax, d, P2);
  value x, a, m, nmax, d; integer m, nmax, d; real x, a;
  array P2;
comment This procedure evaluates to d significant digits the
  Legendre functions P_{a+n}^m(x) for fixed x > 1, a, m \ge 0, and for
  n = 0(1)nmax. The results are stored in the array P2. They are
```

$$P^m_{a+n+1}(x) = \frac{2n+2a+1}{n+a-m+1} x P^m_{a+n}(x) - \frac{n+a+m}{n+a-m+1} P^m_{a+n-1}(x),$$

the initial values being calculated with the help of the procedure Legendre 1;

begin integer n; array P1[0:m]; if m < 0 then go to alarm; $Legendre\ 1(x, a, m, d, P1)$; P2[0] := P1[m]; if nmax > 0 then begin $Legendre\ 1(x, a+1, m, d, P1)$; P2[1] := P1[m] end; for n := 1 step 1 until nmax-1 do $P2[n+1] := ((2\times n+2\times a+1)\times x\times P2[n] - (n+a+m)\times P2[n-1])/(n+a-m+1)$ end $Legendre\ 2$;

procedure conical (x, tau, nmax, d, P);

obtained recursively from

value x, tau, nmax, d; integer nmax, d; real x, tau; array P; comment This is an adaption of the procedure $Legendre\ 1$ to the case $\alpha = -\frac{1}{2} + i\tau$, where τ is real. The procedure thus generates Mehler's conical functions $P^n_{-\frac{1}{2}+i\tau}(x)$ to d significant digits for n = 0(1)nmax and x > 1. The results are stored in the array P. To avoid excessively large and excessively small numbers, we let $f_n = P^n_{-\frac{1}{2}+i\tau}(x)/n!$ and first compute f_n from the recurrence relation

$$f_{n+1} + \frac{2nx}{(n+1)(x^2-1)^{\frac{1}{2}}} f_n + \frac{(n-\frac{1}{2})^2 + \tau^2}{n(n+1)} f_{n-1} = 0,$$

and the identity

$$f_0 + \sum_{n=1}^{\infty} \lambda_n f_n = [x + (x^2 - 1)^{\frac{1}{2}}]^{-\frac{1}{2}} \cos (\tau \ln [x + (x^2 - 1)^{\frac{1}{2}}]),$$

where

$$\lambda_n = n! \left[\frac{\Gamma(\frac{1}{2} + i\tau)}{\Gamma(\frac{1}{2} + i\tau + n)} + \frac{\Gamma(\frac{1}{2} - i\tau)}{\Gamma(\frac{1}{2} - i\tau + n)} \right].$$

The \(\lambda\)'s are obtained recursively by

$$\lambda_1 = rac{1}{rac{1}{4} + au^2}, \qquad \lambda_2 = rac{3 - 4 au^2}{(rac{1}{4} + au^2) \, (rac{9}{4} + au^2)},$$

$$\lambda_{n+1} = \frac{1 + \frac{1}{n}}{\left(1 + \frac{1}{2n}\right)^2 + \left(\frac{\tau}{n}\right)^2} (2\lambda_n - \lambda_{n-1}) \qquad (n = 2, 3, \dots).$$

```
specified by d is too stringent the procedure may not converge
  at all due to the accumulation of rounding errors;
begin integer n, nu, m; real epsilon, t, x1, x2, sum, lambda 1,
  lambda 2, lambda, r, s; array Papprox, Rr[0:nmax];
  if x < 1 \lor nmax < 0 then go to alarm;
  if x = 1 then
  begin
    P[0] := 1; for n := 1 step 1 until nmax do P[n] := 0;
  go to L3
  end;
  t := tau \uparrow 2;
  for n := 0 step 1 until nmax do Papprox[n] := 0;
  epsilon := .5 \times 10 \uparrow (-d);
  x1 := sqrt(x \uparrow 2 - 1); \quad x2 := x + x1;
  sum := cos(tau \times ln(x2))/sqrt(x2); \quad x1 := 2 \times x/x1;
  nu := 30 + entier ((1+(.140+.0246 \times tau) \times (x-1)) \times nmax);
L0: n := 2;
  lambda \ 1 := 1/(.25+t);
  lambda \ 2 := (3-4\times t)/((.25+t)\times (2.25+t));
L1: lambda := (1+1/n) \times (2 \times lambda \ 2 - lambda \ 1)/
  ((1+.5/n)\uparrow 2 + (tau/n)\uparrow 2);
  if n < nu then
  begin
  lambda \ 1 := lambda \ 2; \quad lambda \ 2 := lambda;
    n := n + 1; go to L1
  end:
  r := s := 0;
L2: r := -((1-.5/n))(2+(tau/n))(2)/(x1+(1+1/n)\times r);
  s := r \times (lambda \ 2+s);
  if n \leq nmax then Rr[n-1] := r;
  lambda 1 := lambda 2;
  lambda \ 2 := 2 \times lambda \ 2 - ((1+.5/n)) + (lau/n)
    \times lambda/(1+1/n);
  lambda := lambda 1;
  n := n - 1; if n \ge 1 then go to L2;
  P[0] := sum/(1+s);
  for n := 0 step 1 until nmax - 1 do P[n+1] := Rr[n] \times P[n];
  for n := 0 step 1 until nmax do
    if abs (P[n]-Papprox[n]) > epsilon \times abs(P[n]) then
    begin
      for m := 0 step 1 until nmax do Papprox[m] := P[m];
      nu := nu + 60; comment To avoid an infinite loop in
         case of divergence the user should provide for an upper
         bound on nu, say 1000, and exit from the procedure when
         nu exceeds this bound, printing an appropriate error
        message:
      go to L0
    end;
  t := 1;
  for n := 1 step 1 until nmax do
  begin
    t := n \times t; P[n] := t \times P[n]
  end;
L3: end conical;
procedure toroidal (x, m, nmax, d, Q);
  value x, m, nmax, d; integer m, nmax, d; real x; array Q;
comment This procedure generates to d significant digits the
  toroidal functions of the second kind, Q_{-1+n}^m(x), for n=0(1)
```

The procedure converges rather slowly if x and τ are both large

(see the graphs in §6 of [2]). If the accuracy requirement as

zero. The method of computation is based on the recurrence

relation $(n-m+\frac{1}{2})Q_{-\frac{1}{2}+n+1}^m(x) - 2nxQ_{-\frac{1}{2}+n}^m(x) + (n+m-\frac{1}{2})Q_{-\frac{1}{2}+n-1}^m(x) = 0,$

nmax, where x > 1, and m is an integer, positive, negative or

$$Q_{-\frac{1}{2}}^m(x) + 2\sum_{n=1}^{\infty} Q_{-\frac{1}{2}+n}^m(x) = (-1)^m \sqrt{\frac{\pi}{2}} \Gamma(m+\frac{1}{2})(x-1)^{-\frac{1}{2}} \left(\frac{x+1}{x-1}\right)^{m/2},$$

and the identity

to which a variant of J. C. P. Miller's backward recurrence algorithm is applied. (See [2] for more details.) The convergence of this procedure is slow for x near 1, and improves rapidly as xincreases;

begin integer n, nu, p; real epsilon, x1, c, sum, r, s; array Qapprox, Rr[0:nmax]; if $x \leq 1 \vee nmax < 0$ then go to alarm; for n := 0 step 1 until nmax do Qapprox[n] := 0; $epsilon := .5 \times 10 \uparrow (-d);$ c := 2.2214414691;if $m \ge 0$ then for n := 0 step 1 until m-1 do $c := -(n+.5) \times c$ for n := 0 step -1 until m+1 do c := -c/(n-.5); $sum := c \times ((x+1)/(x-1)) \uparrow (m/2)/sqrt(x-1); \quad x1 := 2 \times x;$ $nu := 20 + entier ((1.15 + (.0146 + .00122 \times m)/(x-1)) \times nmax);$ $L0: \quad r := s := 0;$ for n := nu step -1 until 1 do begin $r := (n+m-.5)/(n \times x1 - (n-m+.5) \times r); \quad s := r \times (2+s);$ if $n \leq nmax$ then Rr[n-1] := rend; Q[0] := sum/(1+s);for n := 0 step 1 until nmax - 1 do $Q[n+1] := Rr[n] \times Q[n]$; for n := 0 step 1 until nmax do if $abs(Q[n]-Qapprox[n]) > epsilon \times abs(Q[n])$ then begin

end end toroidal;

nu := nu + 10; go to L0

comment All procedures were tested on the CDC 3600 computer. Some of the tests that were run are described below;

for p := 0 step 1 until nmax do Qapprox[p] := Q[p];

comment The procedures integer Legendre 1-3 were driven to print test values to 6 significant digits of $P_{n}^{m}(x)$, $Q_{m}^{n}(x)$, $Q_{n}^{m}(x)$, m = 0(1)10, for x = 1.5, 3, 10, and n = 0(1)5. As far as possible, the results were compared with values tabulated in [5], and found to be in complete agreement. Similarly, test values of $P_{-\frac{1}{2}+n}^{m}(x)$, m=0(1)4, were obtained from the procedure Legendre 1, for x = 1.5, 3, 10, and n = 0(1)5. All agreed with values tabulated in [5]. More extensive tests could be run by having the procedure "verify" the addition theorem

$$\begin{split} P_{\alpha}(xy-\sqrt{(x^2-1)}\sqrt{(y^2-1)}) &= P_{\alpha}(x)P_{\alpha}(y) \\ &+2\sum_{m=1}^{\infty}(-1)^m\frac{\Gamma(\alpha-m+1)}{\Gamma(\alpha+m+1)}P_{\alpha}{}^m(x)P_{\alpha}{}^m(y), \quad x>1, y>1; \end{split}$$

comment The procedure conical (with d=6) was run to produce test values of $P_{-k+i\tau}^m(x)$, m=0, 1, for x=1.5, 5, 10, 20, and $\tau = 0(10)30$. The results agreed to 6 significant digits with those in [10], [11];

comment The procedure toroidal was driven to generate test values to 6 significant digits of $Q_{-\frac{1}{2}+n}^m(x)$, $Q_{-\frac{1}{2}+n}^{-m}(x)$, n=0(1)5, for x = 1.5, 3, 10, and m = 0(1)4. All values of $Q_{-\frac{1}{2}+n}^{m}(x)$ were checked against those in [5]. There were no discrepancies. The values of $Q_{-\frac{1}{2}+n}^{-m}(x)$ were compared with those of $[\Gamma(n-m+\frac{1}{2})/$ $\Gamma(n+m+\frac{1}{2})]Q_{-\frac{1}{2}+n}^m(x)$. The largest relative error observed was $1.5_{10} - 9$, occurring at m = 4, n = 5, x = 1.5;

comment Integrals of the form

$$f_n(k^2, \alpha) = (-1)^n \int_0^{\pi/2} [1 - k^2 \sin^2 \psi]^{\alpha} \cos 2n\psi \ d\psi, \quad 0 < k < 1,$$

are repeatedly encountered in applied mathematics (see, e.g., [6]-[9], where $\alpha = -\frac{3}{2}$, or $\alpha = -\frac{5}{2}$). It is readily seen that

$$f_n(k^2, \alpha) = (-1)^n \frac{\pi}{2} \frac{\Gamma(\alpha+1)}{\Gamma(\alpha+n+1)} (1 - k^2)^{\alpha/2} P_{\alpha}^n \left(\frac{2 - k^2}{2\sqrt{(1-k^2)}} \right).$$

The program that follows generates $(1-k^2)f_n(k^2, \alpha)$, n =0(1)10, for $\alpha = -\frac{3}{2}$, $-\frac{5}{2}$, and $k^2 = .1$, .5, .9, calling for an accuracy of 6 significant digits. Selected results are shown below.

Those for $\alpha = -\frac{3}{2}$ were compared with values tabulated in [6].

There was agreement in all four decimal places given;

```
begin integer n; real alpha, k2, c; array P1[0:10];
  for alpha := -1.5, -2.5 do
  for k2 := .1, .5, .9 do
      c := 1.570796327 \times (1-k2) \uparrow (1+alpha/2);
      Legendre 1 (.5 \times (2-k2)/sqrt(1-k2), alpha, 10, 6, P1);
      for n := 0 step 1 until 10 do
        P1[n] := c \times P1[n]; \quad c := -c/(n+alpha+1);
        outreal (1, P1[n])
      end
    end;
  go to skip;
alarm: outstring (1, 'parameters not in range');
skip: end:
comment The integrals
```

 $\Omega_j(k) = \int_0^{\pi} (1 - k^2 \cos \phi)^{-\frac{1}{2}-j} d\phi, \quad 0 \le k < 1, j = 0, 1, 2, \cdots$

arose in recent radiation field studies ([1]). One has

$$\Omega_{j}(k) = \pi (1-k^{4})^{-(\frac{1}{2}+j)/2} P_{-\frac{1}{2}+j}((1-k^{4})^{-\frac{1}{2}}).$$

The program below calculates $\Omega_i(k)$ to 8 significant digits for $k^2 = .2(.2).8$, j = 0(1)9. The results agree to 8 figures with the values tabulated in [1];

begin integer j; real k2, x, x1; array P2, omega [0:9]; for k2 := .2 step .2 until .9 do begin $x := 1/sqrt(1-k2\uparrow 2);$ Legendre 2(x, -.5, 0, 9, 8, P2); $x1 := 3.1415926536 \times sqrt(x);$ omega $[0] := x1 \times P2[0];$ for j := 1 step 1 until 9 do $x1 := x \times x1$; $omega[j] := x1 \times P2[j]$ for j := 0 step 1 until 9 do outreal (1, omega[j])end: go to skip; alarm: outstring (1, 'parameters not in range'); skip: end

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end

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ALGORITHM 260

6-J SYMBOLS [Z]

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real procedure SJS (J1, J2, J3, L1, L2, L3, factorial); value J1, J2, J3, L1, L2, L3; integer J1, J2, J3, L1, L2, L3; array factorial;

comment SJS calculates the 6-j symbols defined by the following formula

where

$$\Delta(a, b, c) = \left[\frac{(a+b-c)! (a-b+c)! (-a+b+c)!}{(a+b+c+1)!} \right]^{\frac{1}{2}}$$

and where j1 = J1/2, j2 = J2/2, j3 = J3/2, l1 = L1/2, l2 = L2/2 l3 = L3/2. [Reference formula 6.3.7 page 99 of EDMONDS, A. R. Angular momentum in quantum mechanics. In *Investigations in Physics*, 4, Princeton U. Press, 1957]. The parameters of the procedure J1, J2, J3, L1, L2, L3 are interpreted as being twice their physical value, so that actual parameters may be inserted as integers. Thus to calculate the 6-j symbol

$$egin{pmatrix} 2 & 2 & 0 \ 2 & 2 & 0 \end{pmatrix}$$

the call would be SJS (4, 4, 0, 4, 4, 0, factorial). The procedure checks that the triangle conditions for the existence of a coefficient are satisfied and that j1+j2+j3, j1+l2+l3, l1+j2+l3 and l1+l2+j3 are integral. If the conditions are not satisfied the value of the procedure is zero. The parameter factorial is an array containing the factorials from 0 up to at least 1+ largest of j1+j2+j3, j1+l2+l3, l1+j2+l3 and l1+l2+j3. Since in actual calculations the procedure SJS will be called many times it is more economical to have the factorials in a global array rather than compute them on every

```
entry to the procedure. The notation is consistent with that
used in the procedure for calculating Vector-coupling coeffi-
cients. See Algorithm 252, Vector Coupling or Clebsch-Gordan
Coefficients [Comm. ACM 8 (Apr. 1965), 217];
begin integer w, wmin, wmax;
real omega;
real procedure delta (a, b, c);
  value a, b, c;
  integer a, b, c;
begin delta := sqrt (factorial [(a+b-c) \div 2]
  \times factorial [(a-b+c) \div 2]
  \times factorial [(-a+b+c) \div 2]/factorial [(a+b+c+2) \div 2])
end delta;
if J1 + J2 < J3 \lor abs(J1 - J2) > J3 \lor J1 + J2 + J3 \neq
  2 \times ((J1+J2+J3) \div 2)
\bigvee J1 + L2 < L3 \bigvee abs(J1 - L2) > L3 \bigvee J1 + L2 + L3 \neq 2 \times 1
  ((J1+L2+L3) \div 2)
((L1+J2+L3) \div 2)
\bigvee L1 + L2 < J3 \bigvee abs(L1 - L2) > J3 \bigvee L1 + L2 + J3 \neq 2 \times J3 
  ((L1+L2+J3)\div 2)
then SJS := 0 else
begin
  omega := 0;
  wmin := J1 + J2 + J3;
  if wmin < J1 + L2 + L3 then wmin := J1 + L2 + L3;
  if wmin < L1 + J2 + L3 then wmin := L1 + J2 + L3;
  if wmin < L1 + L2 + J3 then wmin := L1 + L2 + J3;
  wmax := J1 + J2 + L1 + L2;
  if wmax > J2 + J3 + L2 + L3 then wmax := J2 + J3 +
    L2 + L3;
  if wmax > J3 + J1 + L3 + L1 then wmax := J3 + J1 +
    L3 + L1;
  for w := wmin \text{ step } 2 \text{ until } wmax \text{ do}
  omega := omega + (if w = 4 \times (w \div 4) then 1 else - 1)
    \times factorial [w \div 2+1]/(factorial [(w-J1-J2-J3) \div 2]
    \times factorial [(w-J1-L2-L3) \div 2]
    \times factorial [(w-L1-J2-L3)\div 2]
    \times factorial [(w-L1-L2-J3) \div 2]
    \times factorial [(J1+J2+L1+L2-w)\div 2]
    \times factorial [(J2+J3+L2+L3-w)\div 2]
    \times factorial [(J3+J1+L3+L1-w)\div 2]);
  SJS := delta (J1, J2, J3) \times delta (J1, L2, L3)
    \times delta (L1, J2, L3) \times delta (L1, L2, J3) \times omega;
```

ALGORITHM 261

end

end SJS

9-J SYMBOLS [Z]

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real procedure NJS(J11, J12, J13, J21, J22, J23, J31, J32, J33, factorial);

value J11, J12, J13, J21, J22, J23, J31, J32, J33; integer J11, J12, J13, J21, J22, J23, J31, J32, J33; array factorial;

comment NJS calculates the 9-j symbols defined by the following formula

j22 = J22/2, j23 = J23/2, j31 = J31/2, j32 = J32/2, j33 = J33/2 [Reference formula 6.4.3 page 101 of Edmonds, A. R. Angular momentum in quantum mechanics. In *Investigations in Physics*, 4, Princeton U. Press, 1957]. The parameters of the procedure J11, J12, J13, J21, J22, J23, J31, J32, J33 are interpreted as being twice their physical value, so that actual parameters may be inserted as integers. Thus to calculate the 9-j symbol

```
    \begin{cases}
      2 & 2 & 0 \\
      2 & 2 & 0 \\
      0 & 0 & 0
    \end{cases}
```

the call would be NJS (4, 4, 0, 4, 4, 0, 0, 0, 0, 0, factorial). The procedure checks that the triangle conditions for the existence of a coefficient are satisfied and that j11+j21+j31, j21+j22+j23, j31+j23+j33 are integral. If the conditions are not satisfied the value of the procedure is zero. The parameter factorial is an array containing the factorials from 0 up to at least 1+ largest of j11+j21+j31, j21+j22+j23, j31+j32+j33, j11+j12+j13, j12+j22+j32, j13+j23+j33. The procedure makes use of the procedure SJS [Algorithm 260, 6-j symbols, Comm. ACM 8 (Aug. 1965), 492], for calculating 6-j symbols;

```
begin integer k, kmin, kmax;
  real NJ;
  if J11 + J21 < J31 \lor abs(J11-J21) > J31 \lor J11 + J21 +
   J31 \neq 2 \times ((J11+J21+J31) \div 2)
  \bigvee J21 + J22 < J23 \bigvee abs(J21-J22) > J23 \bigvee J21 + J22 +
   J23 \neq 2 \times ((J21+J22+J23) \div 2)
  \bigvee J31 + J32 < J33 \bigvee abs(J31-J32) > J33 \bigvee J31 + J32 +
   J33 \neq 2 \times ((J31+J32+J33) \div 2)
  \lor J11 + J12 < J13 \lor abs(J11-J12) > J13 \lor J11 + J12 +
   J13 \neq 2 \times ((J11+J12+J13) \div 2)
  \lor J12 + J22 < J32 \lor abs(J12-J22) > J32 \lor J12 + J22 +
   J32 \neq 2 \times ((J12 + J22 + J32) \div 2)
  \bigvee J13 + J23 < J33 \bigvee abs(J13-J23) > J33 \bigvee J13 + J23 +
   J33 \neq 2 \times ((J13+J23+J33) \div 2)
  then NJS := 0 else
  \mathbf{begin}\ NJ := 0;
   kmin := abs(J21-J32);
    if kmin < abs(J11-J33) then kmin := abs(J11-J33);
    if kmin < abs(J12-J23) then kmin := abs(J12-J23);
      kmax := J21 + J32;
    if kmax > J11 + J33 then kmax := J11 + J33;
    if kmax > J12 + J23 then kmax := J12 + J23;
      for k := kmin \text{ step } 2 \text{ until } kmax \text{ do}
    NJ := NJ + (if k=2 \times (k+2) then 1 else -1) \times (k+1) \times
      SJS(J11, J21, J31, J32, J33, k, factorial) \times
      SJS(J12, J22, J32, J21, k, J23, factorial) \times
      SJS(J13, J23, J33, k, J11, J12, factorial);
    NJS := NJ
  end
```

ALGORITHM 262

end NJS

NUMBER OF RESTRICTED PARTITIONS OF N

J. K. S. McKay (Recd. 7 Dec. 1964 and 9 Mar. 1965) Computer Unit, University of Edinburgh, Scotland

procedure set (p, N); integer N; integer array p; comment The number of partitions of n with parts less than or equal to m is set in p[n, m] for all n, m such that $N \ge n \ge m \ge 0$.

References:

1. GUPTA, H., GWYTHER, C. E., AND MILLER, J. C. P. Tables of

```
partitions. In Royal Society Mathematical Tables, vol. 4, Cambridge U. Press, 1958.
```

2. HARDY, G. H., AND WRIGHT, E. M. The Theory of Numbers. Ch. 19, 4th ed., Clarendon Press, Oxford, 1960;

```
begin integer m, n;

p[0, 0] := 1;

for n := 1 step 1 until N do

begin p[n, 0] := 0;

for m := 1 step 1 until n do

p[n, m] := p[n, m-1] +

p[n-m, \text{ if } n-m < m \text{ then } n-m \text{ else } m]

end

end set
```

ALGORITHM 263

PARTITION GENERATOR [A1]

J. K. S. McKay (Recd. 7 Dec. 1964 and 9 Mar. 1965) Computer Unit, University of Edinburgh, Scotland.

procedure generate (p, N, position, ptn, length);
integer array p, ptn; integer N, length, position;

comment The partitions of N may be mapped in their natural order, 1-1, onto the consecutive integers from 0 to P(N)-1 where P(N)(=p[N,N]) is the number of unrestricted partitions of N. The array p is set by the procedure set [Algorithm 262, Number of Restricted Partitions of N, Comm. ACM 8 (Aug. 1965), 493]. On entry position contains the integer into which the partition is mapped. On exit length contains the number of parts and ptn[1: length] contains the parts of the partition in descending order.

REFERENCE:

 LITTLEWOOD, D. E. The Theory of Group Characters. Ch. 5, 2nd ed., Clarendon Press, Oxford, 1958;

```
begin integer m, n, psn;
    n := N;    psn := position; length := 0;
A: length := length + 1; m := 1;
B: if p[n, m] < psn then begin m := m + 1; go to B end else
    if p[n, m] > psn then
C: begin
        ptn[length] := m;    psn := psn - p[n, m-1]; n := n - m;
        if n ≠ 0 then go to A; go to D
    end
    else m := m + 1; go to C;
D: end generate
```

ALGORITHM 264

MAP OF PARTITIONS INTO INTEGERS [A1] J. K. S. McKay (Recd. 7 Dec. 1964 and 9 Mar. 1965) Computer Unit, University of Edinburgh, Scotland

```
integer procedure place(p, n, pln); value n;
integer array p, pln; integer n;
comment place is the inverse of the procedure.
```

comment place is the inverse of the procedure generate [Algorithm 263, Partition Generator, Comm. ACM 8 (Aug. 1965), 493]. The array p is set by the procedure set [Algorithm 262, Number of Restricted Partitions of N, Comm. ACM 8 (Aug. 1965), 493]. The procedure produces the integer into which the partition of n, stored in descending order of parts in ptn[1] onwards, is mapped;

```
begin integer j, d;

d := 0;

if n = 0 then go to B;

j := 0;

A: j := j + 1; d := p[n, ptn[j] - 1] + d; n := n - ptn[j];

if n \neq 0 then go to A;

B: place := d

end place
```