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THE NUMERICAL COMPUTATION OF THE CONFLUENT HYPERGEOMETRIC FUNCTION U(a,b,z)

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by

N.M. Temme

ABSTRACT

An algorithm is given for the computation of the confluent hypergeometric function U(a,b,z). For real values of a, b and z, z > 0, ALGOL 60 procedures are given. The computations are based on a Miller algorithm and on asymptotic expansions.

KEY WORDS & PHRASES: confluent hypergeometric function, Kummer function, computation of special functions, Miller algorithm,

ALGOL 60 programs

^{*)} This report will be submitted for publication elsewhere.

1. INTRODUCTION

1.1. Definitions and relevant properties

We consider the computation of the confluent hypergeometric function

(1.1)
$$U(a,b,z) = \frac{1}{\Gamma(a)} \int_{0}^{\infty} e^{-zt} t^{a-1} (1+t)^{b-a-1} dt.$$

This representation is valid for Re a > 0, Re z > 0, b ϵ C. For other values of a and z we define U(a,b,z) by analytic continuation. In general, i.e., for general a and b values, U(a,b,z) is singular at z = 0. It is a many-valued function with respect to z and we consider for $|\arg z| < \pi$ the principal branch, which is real (if a and b are real) for z > 0. With respect to a (or b) U(a,b,z) is an entire function. For a = 0,-1,-2,... it can be written in terms of Laguerre polynomials

(1.2)
$$U(-n,\alpha+1,z) = (-1)^n n! L_n^{(\alpha)}(z)$$
.

If b-a-1 = n (n = 0,1,2,...) it also reduces to an elementary function. It easily follows from (1.1) that

(1.3)
$$U(a,a+n+1,z) = \sum_{k=0}^{n} (a)_{k} {n \choose k} z^{-a-k},$$

where (a)_k = $\Gamma(a+k)/\Gamma(a)$, k = 0,1,2,....

The function U(a,b,z) is a solution of Kummer's equation

$$(1.4)$$
 $zw'' + (b-z)w' - aw = 0.$

A second solution is the function (also denoted by $_1F_1^{}$ (a,b,z))

(1.5)
$$M(a,b,z) = \sum_{n=0}^{\infty} (a)_n/(b)_n z^n/n!$$

which is regular for all finite z-values, although it is undefined for some pairs (a,b).

The functions U(a,b,z) and M(a,b,z) satisfy recurrence relations with

respect to a and b. With respect to a we have

(1.6)
$$f_{a-1} + (b-2a-z)f_a + a(1+a-b)f_{a+1} = 0$$

which is satisfied by

(1.7)
$$U(a,b,z)$$
 and $M(a,b,z)/\Gamma(1+a-b)$.

With respect to b we have

(1.8)
$$(b-a-1)f_{b-1} + (1-b-z)f_b + zf_{b+1} = 0.$$

with solutions

(1.9)
$$U(a,b,z)$$
 and $\Gamma(b-a)/\Gamma(b)M(a,b,z)$.

We use here the notation of ABRAMOWITZ & STEGUN (1964, Chapter 13). More information on Kummer's function can be found in this and in many other references, for instance in SLATER (1960).

For certain combinations of a and b the function U(a,b,z) reduces to other special functions. We list here some examples (see ABRAMOWITZ & STEGUN (1964, p.510) for a more extensive table).

a 	b	Z	relation	function	
V+1/2	2v+1	2z	$\pi^{-\frac{1}{2}} e^{z} (2z)^{-v} K_{v}(z)$	modified Bessel	
-n	α+1	z	$(-1)^n n! L_n^{\alpha}(z)$	Laguerre polynomial	
$1-\alpha$	$1-\alpha$	z	$\left\{ e^{z} \Gamma(\alpha,z) \\ e^{z} e^{-\alpha} \Gamma(\alpha,z) \right\}$	for some 1 of a second	
1	1+α	z	$e^{z}z^{-\alpha}\Gamma(\alpha,z)$	incomplete gamma	
-1 ₂ V	<u>1</u> 2	1 ₅ z ²	$2^{-\frac{1}{2}V}e^{\frac{1}{4}z^2}D_{V}(z)$	parabolic cylinder	

The incomplete gamma function has as special cases the exponential integrals, the sine and cosine integrals and the error functions. $D_n(z)$ is an Hermite polynomial, $D_{-n-1}(z)$ is a repeated integral of the error function

$$(n = 0, 1, 2, ...)$$
.

1.2. Contents of the paper

The algorithms given here can be used for complex values of a,b and z. In order to formulate concrete stability conditions it is better to concentrate on real a,b and z = x > 0.

The algorithms are implemented in two ALGOL 60 procedures:

1. the procedure chu computes the values

(1.10)
$$u_k = (a)_k U(a+k,b,x)$$
 and $(a)_K U'(a+K,b,x)$

for a ≥ 0 , k = 0,1,...,K, b $\in \mathbb{R}$, x > 0 and K is an integer ≥ 0 .

2. the procedure uabx computes the values

$$(1.11)$$
 $U(a,b,x)$ and $U'(a,b,x)$

for $a \in \mathbb{R}$, $b \in \mathbb{R}$, x > 0.

The prime denotes differentiation with respect to x. The single value (a) $_K$ U'(a+K,b,x), delivered by chu is used for a backward recursion process and it plays an important role when chu calls recursively for itself. Also uabx calls for chu, and then the derivative is important too. It is possible to obtain the derivative U'(a+K,b,x) from the values u_K , u_{K-1} , for instance by using

$$xU'(a,b,x) = (a-b+x)U(a,b,x)-U(a-1,b,x)$$
.

For small values of x and/or large values of b this formula is not stable. Our methods in chu guarantee a stable computation for the derivative of U(a+K,b,x).

In Section 2 we discuss recursion with respect to a. For values of x bounded away from zero we can use a Miller algorithm. For x-values close to zero, we use asymptotic expansions. In an earlier publication TEMME (1975a) we used analogous methods for the computation of (1.10) with a = b = 1.

In Section 3 we consider some aspects of recursion with respect to b. The ALGOL 60 procedures are described in Section 4. The procedures call for procedures published earlier in TEMME (1975b), a publication on the computation of modified Bessel functions.

2. RECURSION WITH RESPECT TO a

From (1.6) and (1.7) it follows that $u_{\hat{k}}$ of (1.10) satisfies

(2.1)
$$(a+k-1)u_{k-1} + (b-2a-x-2k)u_k + (a+k+1-b)u_{k+1} = 0$$

with as a second solution

(2.2)
$$g_k = \Gamma(a+k)/\Gamma(1+a+k-b) M(a+k,b,x)$$
.

From asymptotic expansions of the gamma functions and from SLATER (1960, p.80) it follows easily that for $k \, \rightarrow \, \infty$

$$u_{k} = 2/\Gamma(a) (k/x)^{(b-1)/2} e^{x/2} K_{b-1} [2(kx)^{\frac{1}{2}}] [1 + 0(k^{-\frac{1}{2}})],$$

$$(2.3)$$

$$g_{k} = \Gamma(b) (k/x)^{(b-1)/2} e^{x/2} I_{b-1} [2(kx)^{\frac{1}{2}}] [1 + 0(k^{-\frac{1}{2}})],$$

where $I_{\nu}(z)$ and $K_{\nu}(z)$ are modified Bessel functions. For Re kx $\rightarrow \infty$ we obtain by using well known expansions for the Bessel function

$$u_{k} \sim \pi^{\frac{1}{2}}/\Gamma(a) (k/x)^{(b-1)/2} (kx)^{-\frac{1}{4}} \exp[\frac{1}{2}x-2(kx)^{\frac{1}{2}}],$$

$$(2.4)$$

$$g_{k} \sim \frac{1}{2}\pi^{-\frac{1}{2}}\Gamma(b) (k/x)^{(b-1)/2} (kx)^{-\frac{1}{4}} \exp[\frac{1}{2}x+2(kx)^{\frac{1}{2}}].$$

So, in the terminology of GAUTSCHI (1967), u_k is a minimal solution and g_k is a dominant solution of (2.1). Hence the computation of u_{k+1} from u_k , u_{k-1} (using (2.1)) is not stable. If we want to use (2.1) for the computation of $\{u_k\}$ we have to use it backwardly, i.e. from u_k , u_{k+1} we compute u_{k-1} . Backward recursion may be unstable for small k; see §3.2.

2.1. A Miller algorithm for $\{\mathbf{u}_k^{}\}$

As follows from (2.4) we can use a Miller algorithm for the computation of $\{u_k\}$. For details of such an algorithm we refer to GAUTSCHI (1967). As normalization we use

(2.5)
$$\sum_{k=0}^{\infty} m_k u_k = x^{-a}, \qquad m_k = (-1)^k {b-a-1 \choose k}.$$

This relation is easily verified by substituting (1.10) in (2.5) and using (1.1). For x > 0, $a \ge 0$, $b \in \mathbb{R}$ the u_k are non-negative; for $b \le a+1$ all m_k are non-negative. Hence in these cases (it will appear that we can restrict b to [0,1]) the series in (2.5) has non-negative terms, which is important in the numerical procedure. For a = 0 we have $u_0 = 1$, $u_1 = u_2 = \dots = u_K = 0$. For the Miller algorithm we suppose $0 < a \le 1$, other positive a-values need not to be considered.

This algorithm was also used in TEMME (1975b) for the computation of the Bessel function $K_{_{\rm V}}({\bf x})$. For x-values satisfying 1 < x \leq 4, CAMPBELL (1980) modified this algorithm by using the Wronskian relation for the modified Bessel functions. His faster method applies also in the present case. For 1.4 < x \leq 6.5 we use (instead of (2.5)) the normalization

(2.6)
$$U(a,b,x)M'(a,b,x) - U'(a,b,x)M(a,b,x) = \frac{\Gamma(b)}{\Gamma(a)} x^{-b} e^{x}.$$

The M-functions are computed by using (1.5); the rate of convergence of (1.5) is the same as that of the exponential function (a = b).

In (2.6) U, M and M' are positive and U' is negative for a > 0, $b \ge 0$, x > 0. Therefore, (2.6) is stable for the indicated ranges of a, b and x. The Wronskian (2.6) is also used in the case x > 6.5 and a = b. In that case the M-functions are exponentials and (2.6) becomes

$$U(a,a,x) - U'(a,a,x) = x^{-a}$$
.

For small a and/or b the gamma functions in (2.6) are not easy to handle in calculations. In the computer program we combine these functions with M' and U' in such a way that underflow or overflow will never occur when a or b is small.

In the algorithm a different version of (2.1) is used. From (2.1) it is not clear whether backward recursion is stable for small values of k. By introducing

(2.7)
$$v_k = (a)_k U'(a+k,b,x)$$

(compare (1.10)) we obtain the first order (2×2) -system

(2.8)
$$\begin{cases} v_k = v_{k+1} - u_{k+1} \\ u_k = [-xv_{k+1} + (a+k+1+x-b)u_{k+1}]/(a+k) \end{cases}$$

If x > 0, a > 0, $b \in \mathbb{R}$, then v_k is negative. Hence, backward recursion is stable for all $k \ge 0$ if $a+1+x-b \ge 0$. As mentioned earlier, we take $a \in (0,1]$, $b \in [0,1]$ and x > 0. Hence (2.8) is stable for these limited ranges of a and b. Other values of b are treated in Section 3.

The starting value ν in the Miller algorithm is computed as in TEMME (1975b). In fact it is the method of OLVER (1967). We take as starting values

$$\bar{u}_{v} = 1$$
, $\bar{v}_{v} = -2v/[x+(x^{2}+4xv)^{\frac{1}{2}}]$.

This choice follows from approximating the differential equation for y = U'(a,b,x)/U(a,b,x), viz. $x(y'+y^2) + (b-x)y - a = 0$, by putting y' = b = 0.

2.2. Backward recursion with computed starting values

For small values of x, the Miller algorithm is not very efficient to generate u_k of (1.10). As follows from (2.4) the dominance of g_k over u_k becomes rather weak if x is small. For small x we use computed starting values for the recursion (2.8). These values are obtained from asymptotic expansions of U(a,b,x) and U'(a,b,x) for large a, which are valid for small x. Such expansions are given in SLATER (1960, p.80). Similar expansions are derived in TEMME (1979), where for the case of real a, b and x > 0 simple bounds are given for the remainders in the expansions. The

expansions are for N = 1, 2, 3, ...

$$U(a,b,x) = \sum_{n=0}^{N-1} c_n(b,x) \phi_n(a,b,x) + R_N(a,b,x)$$

$$U'(a,b,x) = \sum_{n=0}^{N-1} d_n(b,x) \phi_{n-1}(a,b,x) + T_N(a,b,x)$$

$$(2.9) \qquad \phi_n(a,b,x) = 2e^{x/2}/\Gamma(a) (x/a)^{(n+1-b)/2} K_{n+1-b} [2(ax)^{\frac{1}{2}}]$$

$$c_n(b,x) = \sum_{j=0}^{n} b_j^{(1)} (x) b_{n-j}^{(2)} (b),$$

$$d_n(b,x) = \sum_{j=0}^{n} b_j^{(1)} (x) b_{n-j}^{(3)} (b).$$

The b $_{j}^{(i)}$ are defined by the generating functions (for $\left|\tau\right|$ < π)

$$\exp[x\mu(\tau)] = \sum_{j=0}^{\infty} b_{j}^{(1)}(x)\tau^{j}; \qquad [\tau/(1-e^{-\tau})]^{b} = \sum_{j=0}^{\infty} b_{j}^{(2)}(b)\tau^{j};$$

$$(2.10)$$

$$b_{j}^{(3)}(b) = (1-j/b)b_{j}^{(2)}(b); \qquad \mu(\tau) = 1/\tau - 1/(e^{\tau}-1) - \frac{1}{2}.$$

The function K in ϕ_n is the modified Bessel function. Coefficients $b_j^{(1)}(x)$ and $b_j^{(2)}(b)$ are for $j=0,\ldots,8$ incorporated in the ALGOL 60 program (in fact $b_j^{(2)}(b)/b$); see arrays bx, bb[0:8] in the block announced by "<u>if</u> $x \le 1.4 \ \underline{then}$ ").

The remainders \boldsymbol{R}_{N} and \boldsymbol{T}_{N} are bounded by simple expressions. Let

(2.11)
$$K(d,b,x) = |\sin d|^{-b} \exp[\frac{1}{2}x(1/d+1/|\sin d|)]$$

then, as proved in TEMME (1979), for a > 0, x > 0, $b \ge 0$

$$|R_{N}(a,b,x)| < d^{b-N}K(d,b,x) \phi_{N}(a,b,x)$$
(2.12)
$$|T_{N}(a,b,x)| < d^{b-N+1}K(d,b+1,x) \phi_{N}(a,b+1,x),$$

where d is arbitrary in $[3\pi/2, 2\pi)$.

£

We use the above expansions for the computation of u_k and v_k' for a large value of k (see (1.10) and (2.7)). We fix N; in the computer program we use N=9. Furthermore we take $0 \le b \le 1$. We have to choose $k \ge K$ so large that, given a ϵ (0,1], $b \in [0,1]$, x > 0, $\epsilon > 0$, $d \in [3\pi/2,2\pi)$,

(2.13) (a)
$$_{k}^{1}R_{N}^{(a+k,b,x)} < \varepsilon u_{k}^{1}$$
 and (a) $_{k}^{1}T_{N}^{(a+k,b,x)} < \varepsilon |v_{k}^{1}|$.

The minimal value of k satisfying both inequalities of (2.13) is computed by using inequalities for ϕ_j (a,b,x) as given in TEMME (1979). Also the value of d is computed according to a device given there.

When u_k and v_k are computed we use (2.8) for backward recursion.

2.3. Negative a-values

The integral (1.1) defines U(a,b,z) for Re a > 0. However, as follows from recursion with respect to a, see (1.6), U(a,b,x) is an entire function of a and recursion can be used for the analytic continuation of (1.1) to Re a \leq 0. First values for the recursion can be obtained from the algorithms of Section 2. We give an ALGOL 60 program uabx which computes U(a,b,x) for a \in R, b \in R, x > 0, and the x-derivative. Computation of (1.10) for a < 0 is not attractive due to possible singularities (for negative integer values of a) of the factor $\Gamma(a+k)/\Gamma(a)$. Special values for a = -n, n = 0,1,2,..., follow from (1.2).

For a $\rightarrow -\infty$, b bounded, x > 0 we have

$$U(a,b,x) = \Gamma(\frac{1}{2}b-a+\frac{1}{4})\pi^{-\frac{1}{2}}e^{\frac{1}{2}x}x^{\frac{1}{4}-\frac{1}{2}b}\cos(\chi+a\pi)[1+\theta(-a)^{-\frac{1}{2}}]$$

.
$$M(a,b,x) = \Gamma(b) \pi^{-\frac{1}{2}} e^{\frac{1}{2}X} (-ax)^{\frac{1}{4}-\frac{1}{2}b} \cos(\chi) [1+\theta(-a)^{-\frac{1}{2}}]$$

with $\chi=(2bx-4abx)^{\frac{1}{2}}-\frac{1}{2}b\pi+\frac{1}{4}\pi$. It follows that U(a,b,x) and $M(a,b,x)/\Gamma(1+a-b)$, the two solutions of (1.6), are not dominant with respect to each other. Thence recursion is possible for both solutions in negative a-direction.

We use (2.8) in the form

$$\begin{cases} U'(a,b,x) = U'(a+1,b,x) - U(a+1,b,x) \\ \\ U(a,b,x) = -U'(a+1,b,x) + (a+x+1-b)U(a+1,b,x) . \end{cases}$$

It is not possible to give full-proof conditions for the stability as was done for a > 0. In fact U(a,b,x) and U(a+1,b,x) may have different signs when a < 0. The same remark applies for the derivatives.

When a < 0 and a = b we have the incomplete gamma case, viz.

$$U(-a,-a,x) = e^{X}\Gamma(1+a,x).$$

In that case we can claim stability since we can recur according to the relation

$$e^{X}\Gamma(a+1,x) = ae^{X}\Gamma(a,x) + x^{a}$$

which is stable for increasing (positive) a. In terms of the U-functions the recursion is

$$U(-a,-a,x) = aU(1-a,1-a,x) + xU(1-a,2-a,x)$$

in which the last term is an elementary function (see (1.3)).

3. RECURSION WITH RESPECT TO b

For convergence aspects of the algorithms of the previous section we restricted b to the interval [0,1]. Here we are concerned with the remaining b-values and we will start with b < 0. Throughout this section we suppose that a > 0 and x > 0.

3.1. Negative b-values

The crucial relation is the reflexion formula

(3.1)
$$U(a,b,x) = x^{1-b}U(1+a-b,2-b,x).$$

If b is negative the b-place in the U-function at the right is positive (in fact the reflexion occurs at b=1, for convenience we use it at b=0). In order to compute

$$u_{k} = (a)_{k}U(a+k,b,x), k = 0,...,K,$$

$$(3.2)$$

$$v_{K} = (a)_{K}U'(a+K,b,x)$$

for b < 0 we first compute

Using (3.1) and U'(a,b,x) = -aU(a+1,b+1,x), we write this as

where $v_k = u_k'$ (see (2.7)).

For computing the values in (3.3) we need an algorithm for computing $\{u_k^{}\}$ for b > 1. Details on this point will be discussed in the next subsection.

The values in (3.4) are used to compute the requested \textbf{u}_k . First \textbf{u}_K is computed by using

(3.5)
$$aU(a,b,x) = a(1+a-b)U(a+1,b,x) - xU'(a,b,x)$$

and the reamining $u_k^{}$ (k = K-1,...,0) follow from the second of (2.8). This recursion is stable since $v_k^{}$ and b are negative. Also (3.5) is stable.

REMARK. Instead of (3.3) we might have computed

$$\bar{u}_k = (c)_k U(c+k,2-b,x), \qquad k = 0,...,K, \qquad c = 1+a-b,$$

$$w = (c)_{K} U'(c+K,2-b,x) = -(c)_{K+1} x^{b-2}U(a+K,b-1,x).$$

Then

$$\bar{u}_{k} = \frac{(c)_{k}}{(a)_{k}} x^{b-1} u_{k};$$

hence u_k follows rather straightforward from the computed u_k . However, we need also v_K . This value can be computed from the u_K , u_{K-1} , or w, u_K by using one of the recursions

$$xU'(a,b,x) = (a-b+x)U(a,b,x) - U(a-1,b,x),$$

$$xU'(a,b,x) = (1-b)U(a,b,x) - (1+a-b)U(a,b,-1,x)$$
.

For small values of x and/or large values of -b they are not stable. In the appraoch described earlier all computations are stable.

3.2. The case b > 1

Recursion with respect to b can be done by using

$$(3.6) (b-a-1)U(a,b-1,x) + (1-b-x)U(a,b,x) + xU(a,b+1,x) = 0,$$

of which a second solution is $\Gamma(b-a)/\Gamma(b)M(a,b,x)$. From the series (1.5) it follows that $M(a,b,x) = 1 + O(b^{-1})$ for $b \to \infty$, a and x bounded. From (1.1) it follows that for $b-a-1 \ge 0$ (by using $(1+t)^{b-a-1} \ge 1$)

(3.7)
$$U(a,b,x) > x^{1-b}\Gamma(b-1)/\Gamma(a)$$
.

Hence for the recursion (3.6) the function U(a,b,x) is dominant with respect to the second solution. It follows that recursion in the forward b-direction is stable.

More insight is gained when we use the derivative as in (2.8). Let us write

$$f_{k} = U(a,b+k,x)$$

$$(3.8)$$

$$g_{k} = U'(a,b+k,x).$$

Then the recursion in the b-direction is given by

(3.9)
$$\begin{cases} f_{k+1} = f_k - g_k \\ xg_{k+1} = (k+b)g_k - af_k. \end{cases}$$

Since $f_K > 0$, $g_k < 0$ ($k \ge 0$), (3.9) is a recursion without subtractions (formula (3.6) lacks this property), and hence it is stable.

Suppose we want to compute (1.10) with b > 1. Then we define $b_1 = b - [b]$ and we compute the values

(a)
$$K^{U(a+K,b_1,x)}$$
, (a) $K^{U'(a+K,b_1,x)}$

by using the algorithms of Section 2. Then we use (3.9) for obtaining u_{K} and v_{V} and then (2.8) can be used for the remaining u_{k} (k = K-1,...,0).

As mentioned earlier, (2.8) is stable if a+k+1+x-b is not negative. Large b values may violate this condition and in fact the second of (2.8) is not stable for large b-values. To show this we need the asymptotic relation (compare (3.7))

(3.10)
$$U(a,b,x) \sim x^{1-b} \Gamma(b-1) / \Gamma(a)$$
,

which is valid for $x \to 0$ (b > 1) or $b \to \infty$ (x fixed). Inserting this in the second of (2.8) (with modifications for v_{k+1} and u_{k+1}) we infer that indeed large values will cancel each other in order to obtain a smaller value, especially when k is small. Repeated application of (2.8) is allowed as long as k is so large that a+k+1+x-b is not negative. If a,b and x (and K) are such that for some k this quantity becomes negative, instabilities may arise.

It is not easy to formulate an "if and only if" condition for the stability. The subtraction p-q of two positive numbers (q < p) is harmless if, say, $q < \frac{1}{2}p$. The recursion (2.8) can be done by checking this criterion. However, in the computer program it is convenient to have a priori information on safe k-values. We use simply the above condition: a k-value is safe if a+k+1+x-b is non-negative. Call m the largest value of k that makes a+k+1+x-b negative. Then

(3.11)
$$\{u_{m+1}, u_{m+2}, \dots, u_{K}\}$$

are computed via (2.8) and for

(3.12)
$$\{u_0, \dots, u_m\}$$

we need a different approach.

The value m is defined by

$$(3.13)$$
 m = [b-x-1-a];

if b-x-1-a = [b-x-1-a] then m:=b-x-2-a. It may happen that m<0. In that case all u_k are obtained by (2.8). If $m\geq K$ none of the u_k are obtained by (2.8). In other words, the sets in (3.11) or (3.12) may be empty.

To obtain the values in (3.12) we may suppose that the values

(3.14) (a)
$${}_{j}U(a+j,b_{1},x)$$
, $j = 0,...,m$, $b_{1} = b-[b]$,

are available, together with their derivatives. We can use (3.9) for recursion up to b with

(3.15)
$$f_{k} = (a)_{j} U(a+j,b_{1}+k,x), \quad g_{k} = (a)_{j} U'(a+j,b_{1}+k,x).$$

All these recursions are stable. However, it may be rather expensive, since every element in (3.14) is recurred to the b-level. For an alternative method, which may be much more efficient, we proceed as follows. We start with the element with j=0 in (3.14) and we recur up to b-m. That is, we compute (3.15) with j=0 for $k=0,1,\ldots,\lfloor b\rfloor$ -m, giving

$$f_{[b]-m} = U(a,b-m,x), \quad g_{[b]-m} = U'(a,b-m,x).$$

Next we compute

(3.16)
$$F_{j} = (a)_{j}U(a+j,b-m+j,x), \quad G_{j} = (a)_{j}U'(a+j,b-m+j,x)$$

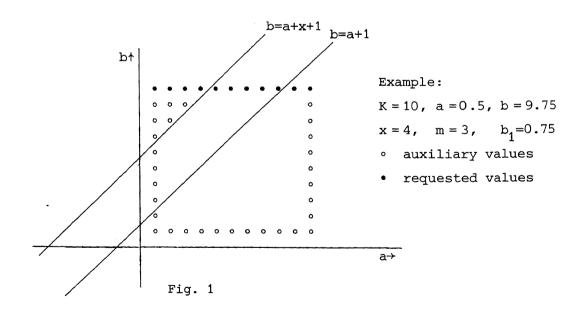
for j=1,2,...,m. (Consider the (a,b)-plane. We compute U and U' along a diagonal in the (a,b)-plane.) These diagonal elements F_j , G_j are obtained by using

(3.17)
$$\begin{cases} aU(a+1,b+1,x) = -U'(a,b,x) \\ axU'(a+1,b+1,x) = -aU(a,b,x) + (b-x)U'(a,b,x), \end{cases}$$

which in fact is Kummer's equation (1.4). In terms of F_{ij} , G_{ij} it reads as

(3.18)
$$\begin{cases} F_{j+1} = -G_{j} \\ xG_{j+1} = -(a+j)F_{j} + (b+j-m-x)G_{j} \end{cases}$$

for j = 0,1,...,m-1. This recursion is stable: G_j is negative and (b+j-m-x) is positive for j = 0,...,m-1; (cf. (3.13). From the diagonal a final recursion in the b-direction is performed by using (3.9) with starting values F_j , G_j in order to obtain (3.12). The procedure is illustrated in Fig. 1.



The values • at the right of the line b = a+x+1 are computed via (2.8).

In the procedure chu this algorithm is controlled by the Boolean variables r and s; $r = \underline{true}$ means that (3.11) is empty, all requested values follow from diagonal elements; $s = \underline{false}$ means that (3.12) is empty, all requested values follow from backward a-recursion. In ALGOL 60 notation : $r := K \le m$, $s := m \ge 0$ (in chu K is replaced by kmax).

3.3. The polynomial case

The actual algorithm for the case b > 1 is more intricate than described above. The point is that we take advantage of the possibility that some or all of the wanted values $\{u_k^{}\}$ are elementary functions. See (1.3). In that case the time-wasting algorithms of Section 2 may be circumvented.

Let us introduce

$$(3.19)$$
 $c = b-a-1$

and we suppose here that c is a non-negative integer. Then the values

(3.20)
$$\{u_0, u_1, \dots, u_c\}$$

are polynomials, and the values

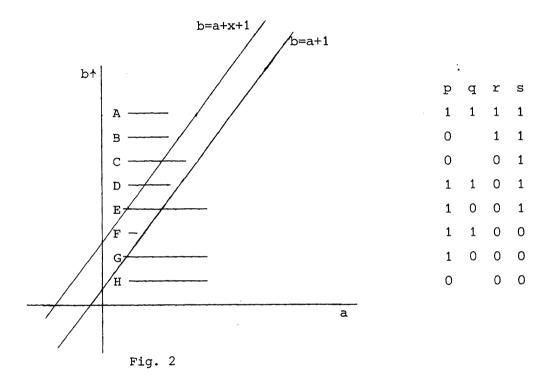
(3.21)
$$\{u_{c+1}, \dots, u_{K}\}$$

are higher transcendentals. The set in (3.21) may be empty. If it is not, its elements are computed as in the previous subsection. Since m (see 3.13) is not larger than c, the set (3.21) is a subset of (3.11). Hence, the higher transcendentals (3.21) can be computed by backward a-recursion, whereas some of the set (3.20) (i.e., $\mathbf{u}_0,\ldots,\mathbf{u}_{\mathbf{m}}$) are to be computed from diagonal elements. These diagonal elements are elementary functions as well. If (3.21) is empty than all $\{\mathbf{u}_k^{}\}$ are polynomials. Then the first $\{\mathbf{u}_0,\ldots,\mathbf{u}_{\mathbf{m}}^{}\}$ are computed from elementary diagonal elements, the remaining with backward a-recursion with elementary starting values.

The polynomial case is recognized in chu by the Boolean variables p and $q: p = \underline{true}$ iff c is a non-negative integer, $p = \underline{true}$ and $q = \underline{true}$ iff

all $\{u_k\}$ are polynomials. That is, if $K \le c$. In ALGOL 60 notation: $p := c = entier(c) \land c \ge 0$, $q := K \le c$.

If we combine the possible cases of §3.2 with those of the present subsection we obtain 8 different situations A,B,...,H. An illustration by means of the (a,b)-plane is again very instructive. In Fig. 2 the positions of the (a,b) parameters of the wanted elements $\{u_k\}$ are depicted with respect to the lines b=a+1, b=a+x+1.



For convenience, $p = \underline{true}$, $p = \underline{false}$, etc. are replaced by p = 1, p = 0, respectively. In the cases A,B,C,D,E diagonal elements must be used (s = 1). In A,B all elements follow from diagonal elements (r = 1). In C,D,E,F,G,H (r = 0) backward a-recursion is used for some (in F,G,H for all) elements. Values of q if p = 0 are not significant; r and s are not independent: s = 0 implies r = 0. G and H are treated as being the same: in G higher transcendentals are used in the backward a-recursion and the process is not terminated at the moment that elementary functions turn up. If K = 0 some cases are equivalent. Then the location with respect to the line b = a + x + 1 is not relevant; the only question is whether it is a polynomial case or not. For

convenience we put r = s = 1 (case A or B) if K = 0.

Examples with numerical values for the different eight cases are given in Table 1.

	a	b	х	K	С	m	
A	2.5	8.5	1.4	2	5	3	_
В	2.0	8.5	1.4	2	5.5	4	
С	2.0	8.5	1.4	5	5.5	4	
D	2.5	8.5	1.4	4	5	3	
E	2.5	8.5	1.4	6	5	3	
F	2.5	8.5	6.5	2	5	-2	
G	2.5	8.5	6.5	6	5	-2	
H	2.0	8.5	6.5	2	5.5	-2	

Table 1

With the shown values of a,b,x,K all cases A through H are covered.

4. ALGOL 60 PROCEDURES

The procedures given here make use of external ALGOL 60 procedures for the computation of the gamma function for positive argument and of the Bessel function $K_{\nu}(x)$, for x>0 and $\nu\in[0,2)$. For the Bessel function we call the procedure given in TEMME (1975b).

4.1. The procedure chu

The heading of the procedure reads as follow:

procedure chu(a,b,x,kmax,eps,u,uprime); value a,b,x,kmax,eps;
real a,b,x,eps,uprime; integer kmax; array u;

The meaning of the formal parameters is:

a,b,x: <arithmetic expressions>;

the parameters of the confluent hypergeometric function U(a,b,x);

 $a \ge 0$, $b < \mathbb{R}$, x > 0.

kmax : <arithmetic expression>;

the upper bound of the array u, $kmax \ge 0$.

eps : <arithmetic expression>;

the desired relative accuracy; eps > 0.

u : <array identifier>

array u[0: kmax];

exit: the values of $\Gamma(a+k)/\Gamma(a)U(a+k,b,x)$, $0 \le k \le kmax$, are

assigned to u[k];

uprime: <identifier>;

exit: the value of $\Gamma(a+kmax)/\Gamma(a)U'(a+kmax,b,x)$ is assigned to

uprime.

The procedure chu calls for the nonlocal procedures besska and gamma; the first is published in TEMME (1975b) (besska also calls for other procedures). The procedure is not protected against underflow or overflow and does not give a message when the parameters are out of range. This last aspect is easily incorporated by the user, the first aspect strongly depends on the computing machinery. In general the functions U(a+k,b,x) are singular at x = 0:

if b < 1, the functions are bounded at x = 0;

if b = 1, $U(a,b,x) = O(\ln x)$ as $x \to 0$;

if b > 1, $U(a,b,x) = O(x^{1-b})$ as $x \to 0$.

Hence for large b-values this singularity may cause overflow. For negative b-values the reflexion formula (3.1) is used. As a consequence, meanwhile an overflow situation may occur. For x-values bounded away from zero together with large b-values see (3.3), which shows that large function values arise in that case too.

If a = 0 we have simply u[0] = 1, u[k] = 0, $k \ge 1$. It follows that values of U(k,b,x) cannot be obtained from

$$U(a+k,b,x) = \frac{\Gamma(a)}{\Gamma(a+k)} u[k]$$

taking a = 0 (except for k = 0). However, by calling the procedure with a = 1, thus calling chu(1, b, x, kmax, eps, u, uprime), we obtain

$$u[k] = \frac{\Gamma(1+k)}{\Gamma(1)} U(1+k,b,x), \qquad k = 0,1,...,kmax,$$

from which the values of U(a,b,x) with positive integer values of a easily follow. Remark that a is not restricted to [0,1].

If kmax or a are very large, underflow will occur in u[k] as can be seen from the first of (2.4).

The (relative) accuracy can be controlled by eps. It is used to control the truncation errors in the approximation processes. Rounding errors are not considered. The may become important, although the recursions in chu are all strictly stable (no significant subtractions). Successive smaller choices of eps may yield worser results, especially if eps is of the same size as the machine accuracy. The relative accuracy in the external procedures hecip gamma and sinh (called by bess ka) is about 10⁻¹⁴.

The user may avoid a call of the Bessel function procedure bess ka (with its external procedures recip gamma and sinh) by skipping the part of the conditional statement announced by $\underline{if}\ x \le 1.4\ \underline{then}$. In that case the procedure will use the Miller algorithm for all x > 0. This will result in a less efficient algorithm with more rounding errors as x becomes smaller.

4.2. The procedure uabx

For convenience we supply a function procedure which gives directly the value of U(a,b,x) for a $\in \mathbb{R}$, b $\in \mathbb{R}$, x>0. This procedure calls for chu of the previous subsection. As a second value it delivers U'(a,b,x).

The heading of the procedure is:

<u>real procedure</u> uabx (a,b,x,eps,uprime); <u>value</u> a,b,x,eps; real a,b,x,eps,uprime;

The meaning of the formal parameters is:

a,b,x: <arithmetic expressions>;
the parameters of U(a,b,x) and U'(a,b,x);

 $a \in \mathbb{R}$, $b \in \mathbb{R}$, x > 0.

eps : <arithmetic expression>;

the desired relative accuracy; eps > 0.

uprime: <identifier>;

exit: the value of U'(a,b,x), the x-derivative of U(a,b,x).

uabx : uabx := U(a,b,x).

For underflow and overflow aspects and the role of eps, see the remarks in the description of chu.

4.3. Testing

The procedures can be compared with existing procedures for the computation of special cases of confluent hypergeometric functions. In this way we checked successfully the modified Bessel functions and the incomplete gamma functions. The procedure chu gives as special case the computation of the repeated integrals of the coerror function. GAUTSCHI (1977) wrote a FORTRAN program for computing

$$i^n \text{ erfc } x = \int_{-\infty}^{\infty} i^{n-1} \text{ erfc t dt,} \qquad n = 1,2,...$$

with i erfc x = erfc x, i⁻¹ erfc x = $(2/\sqrt{\pi})e^{-x^2}$. In terms of the U-functions we have for $x \ge 0$

$$i^{n} \text{ erfc } x = \pi^{-\frac{1}{2}} 2^{-n} e^{-x^{2}} U(\frac{1}{2}n + \frac{1}{2}, \frac{1}{2}, x^{2}),$$

with as special case the error function for n = 0.

The procedures can also be checked against theirselves. The x-interval is divided in 3 subintervals: (0,1.4], (1.4,6.5], $(6.5,\infty)$. With

$$\mathbf{x}_{1}^{\pm} = 1.4(1 \pm \delta), \quad \mathbf{x}_{2}^{\pm} = 6.5(1 \pm \delta)$$

we computed $U(a,b,x_1^{\pm})$ and $U(a,b,x_2^{\pm})$ and we compared the results with each other. We also compared U(a,a+n+1,x) with $U(a(1+\delta),a+n+1,x)$ (δ somewhat larger than the machine accuracy; the computer should recognize the poly-

nomial case in U(a,a+n+1,x) and the non-polynomial case in $U(a(1+\delta),a+n+1,x)$). All tests were satisfactory. They were done on the CD CYBER 73 of SARA, Amsterdam (machine accuracy 2^{-48}).

The boundary points 1.4 and 6.5 for the x-intervals were obtained by comparing computing time for the following choice of the parameters in uabx

$$a = .32$$
, $b = .56$, eps = 10^{-10} .

In the immediate neighbourhood of x = 1.4 the computing time was about 0.02 s, at x = 6.5 it was 0.03 s. A call of chu with large values of kmax and |b| will require much more computing time.

Finally we give the starting index v for the Miller algorithm for a = .5, b = 1, $eps = 10^{-12}$, kmax = 0 and for several values of x:

4.4. Codes of chu and uabx

```
procedure chu(a,b,x,kmax,eps,u,uprime); value a,b,x,kmax,eps;
real a,b,x,eps,uprime; integer kmax;
                                         array u;
comment computes gamma(a + k) / gamma(a) \times u(a + k, b, x)
for k=0 (1) kmax, and the x-derivative of u(a+kmax,b,x)
if a<0 or x<0 or kmax<0 or eps<0 then
        comment here the user can incorporate an output statement
begin
  with the message "parameters out of range"
end else
if a=0 then
begin u[0]:=1; uprime:= 0;
        kmax := kmax  step -1  until  1  do  u[kmax] := 0
   for
end else
if b<0 then
        real c,d,e,w; integer j; array v[0:kmax];
begin
   c := a-b+1; d := x+(-b); chu(c,l-b,x,kmax,eps,v,w);
        j:= 0 step 1 until kmax do
   begin e:=(a+j)\times d; v[j]:=-e\times v[j]; d:=e/(c+j) end;
   uprime:= v[kmax]; u[kmax]:= -x×(uprime+e×w)/(a+kmax);
   c := c+x; for j := kmax-1  step -1  until 0  do
   u[j] := (-x \times v[j+1] + (c+j) \times u[j+1])/(a+j)
```

```
else
end
if b>l then
        real al,bl,c,d,e,f,g,h,u3,v,w; integer i,j,k,m,n;
begin
   boolean p,q,r,s;
   procedure brec(a,b,k,f,g); value a,b,k; real a,b,f,g;
                                integer
                                        k;
                                          until k
   begin k:=k-1; for
                         i:=0 step
                                      1
      begin h:= f-g; g:= ((i+b)\times g-a\times f)/x; f:= h end
   n:= entier(b); bl:= b-n; al:= a+kmax; c:= b-a-1;
   e:= c-x; m:= entier(e); if m=e then m:= m-1;
   p:= c=entier(c) and c>0; q:= kmax\langlec; r:= kmax\langlem; s:= m\rangle0;
       kmax=0 then r:=s:= true;
   if
                m:= kmax; k:= (if p then
                                                else
                                                       n)-m;
          then
                                             С
       ٦r
           then
   if
   begin
          if p and q then
      begin g:= 1; i:= kmax-1; for
                                      j:= 0 step l until i do
         g := g \times (j+a); f := g \times x + (-a1); g := -a1 \times f/x;
         brec(al,al+l,c-kmax,f,g)
          else
      end
      begin chu(a,bl,x,kmax,eps,u,u3); f:=u[kmax]; g:=u3;
         brec(al,bl,n,f,g); if \neg p and s then
         begin for j:= kmax srep -1
                                          until
            u3:=u3-u[j]; v:=u[0]; w:=u3; d:=b1
         end
      end; n:= m+1; u[kmax]:= f; uprime:= g; if \neg s then
           j:= kmax-1 step -1 until n do
      begin h:=(-x\times g+(j-e)\times f)/(a+j); g:=g-f; f:=u[j]:=h end
   end; if s then
          if p then
   begin
      begin v:=x\uparrow(-a); w:=-a\times v/x; d:=a+1
                                             end
            then
      begin chu(a,b1,x,0,eps,u,w); v:=u[0]; d:=b1
      brec(a,d,k,v,w); e:= b-n-x;
            j := 0 step 1 until m do
      for
      begin
             if j=0 then
        begin f:= u[0]:= v; g:= w end else
         <u>begin</u> h:= -w; g:= w:= -((a+j-1)×v-(j+e)×w)/x; v:= u[j]:= h
         end; brec(a+j,b+j-m,m-j,u[j],g)
      end; if m=kmax then uprime:= g
   end
end else
if x \leq 1.4
            then
begin real d,delta,e,f,p,q,r,s,t,t0,t1,u0,u1,u2,u3,v,w,x2,y,z;
          n,nu,k0,k1,i,j; <u>array</u> bb,bb1,bx[0:8],fi[-1:8];
   integer
  n := 9;
```

```
v := 12.56637; r := (x-v \times (b+1))/2; d := (v \times n + r - sqrt(r \times r + 4 \times n \times x))/(2 \times n);
      if d < 4.7124 then
                 d:=4.7\overline{124}; v:=w:=1 end else
      begin
                 v := abs(sin(d)); w := v + (-1-b) end;
      begin
      w:= w \times exp(.5 \times x \times (1/v+1/d));
      delta:= eps \times exp(-.5 \times x + (n-1-b) \times ln(d))/w;
      z := .5/de1ta; v := .5-b; i := n-1;
                j:=1 step 1 until i do z:=z\times(j+v); i:=0;
      for
      t:= sqrt(x)\times z\uparrow(1/(2\times n)); e:= ln(delta)+n-n\times ln(x);
lab: r := n+b+t; s := 1+b+t; p := 1n(r); q := 1n(s);
      f := (ln(t+.5)-2 \times n \times ln(t)+(r-.5) \times p-(s-.5) \times q-e)/
            (1/(t+.5)-2\times n/t+.5\times (n-1)/(r\times s)+p-q);
            f<0 then
      begin
                 t := t-f; t := sqrt(2 \times x + t \times t); i := i+1;
                 i<10 then
                                    goto
      end else
                     k0 := 1 + entier(t \times t/x - a);
      nu:= if kmax>k0 then l+kmax else
      r := a + nu; w := sqrt(x/r); v := 2 \times r \times w;
       bess ka(-b,v,t0,t1);
       v := w + (-b); bb[0] := bb1[0] := bx[0] := 1;
      u1:= fi[-1]:= v \times t0; u0:= fi[0]:= v \times w \times t1; x2:= x \times x;
      bx[1] := -x/12;
       bx[2] := x2/288;
       bx[3] := -x \times (5 \times x^2 - 7^2) / 51840;
       bx[4] := x2 \times (5 \times x2 - 288) / 2488320;
       bx[5] := -x \times (x2 \times (7 \times x2 - 1008) + 6912) /
                                                               209018880;
       bx[6] := x2 \times (x2 \times (35 \times x2 - 10080) + 279936) / 75246796800;
       bx[7] := -x \times (x2 \times (x2 \times (x2 \times 5 - 2520) + 176256) - 746496) / 902961561600;
       bx[8] := x2 \times (x2 \times (x2 \times (x2 \times (x2 \times 5 - 4032) + 566784) - 9953280) / 86684309913600;
       bb[1] := .5;
       bb[2] := (3 \times b-1)/24;
       bb[3] := b \times (b-1)/48;
       bb[4] := (b \times (b \times (b \times 15 - 30) + 5) + 2) / 5760;
       bb[5] := b \times (b \times (b \times (b \times 3-10)+5)+2)/11520;
       bb[6] := (b \times (b \times (b \times (b \times (b \times 63 - 315) + 315) + 91) - 42) - 16)/2903040;
       bb[7] := b \times (b \times (b \times (b \times (b \times (b \times 9 - 63) + 105) + 7) - 42) - 16) / 5806080;
       bb[8] := (b \times 135 - 1260) + 3150) - 840) - 2345) -
                    540)+404)+144)/1393459200;
       for
                i:= 1 step 1 until
                                                n-1
       begin
           t0:= bb[i]; t1:= bb1[i]:= (b-i)\times t0;
           for
                    j := 1
                                     1
                             step
                                           until
                                                     i-1
           begin
```

```
t0:=t0+bb[i-i]\times bx[i];
          t1:= t1 + bb1[i-j] \times bx[j]
       end;
       t0:= bx[i]+b\times t0; t1:= t1+bx[i];
       fi[i] := (x \times fi[i-2] + (i-b) \times fi[i-1])/r;
       u0:=u0 + t0 \times fi[i]; u1:=u1 + t1 \times fi[i-1]
   end;
   w := 2 \times \exp(x/2) / \operatorname{gamma}(1+a);
   u2:= w \times u0; u3:= -w \times u1; v:= a+1-b+x; k1:= nu-1;
          j:= kl step -l until l do
   begin ul:= (-x \times u3 + (v+j) \times u2)/(a+j);
                                     j<kmax then
       u3:=u3-u2; u2:=u1;
                                if
                                                       u[j] := a \times u2;
       if j=kmax then
                           uprime:= a×u3
   end; u[0] := -x \times u3 + v \times u2;
   if kmax=0 then uprime:= a \times (u3-u2)
end else
begin
         real ar, br, cr, c, er, m0, m1, mr, p0, p1, p2, q, u1, u2, u3, v, w;
   integer k,n,r; boolean large x;
   procedure recursion;
   begin p2:= (brxpl-arxp0)/cr; er:= erxar/cr;
       r:= r+1; if large x then mr:= mr \times (1+c/r); v:= er/p2;
       br:= br+2; cr:= cr+1; p0:= p1; p1:= p2
   end recursion;
   n:= entier(a); <u>if</u>
                          a=n then n:=n-1; a:=a-n; kmax:=kmax+n;
   large x:= x>6.5 and a\neq b;
   if large x then mr:= 1 else
   begin mr:= 0; if a=b then
       begin m0:=a; m1:=1 end
                                        else
       begin m0:= 0; m1:= v:= 1;
                 r := 1, r+1  while v \ge m1 \times eps
          for
                                                  do
                  v := v \times x/r; m0 := m0+v; v := v \times (a+r)/(b+r); m1 := m1+v
          begin
          v := \exp(-x) \times \operatorname{gamma}(a+1) / \operatorname{gamma}(b+1);
          m0 := v \times (b+a \times m0); m1 := v \times m1
       end
   end;
   c:=a-b; cr:=2+c; br:=x+a+cr; p0:=0;
   v := p1 := er := 1; r := 0;
   for ar:= a+r while r< kmax do recursion; w:= p0 \times p1/er;
   for ar:= a+r, ar+1 while v\times(w/p0+mr\times(2+a/r)) eps do recursion;
   c := 1+c; v := x+c; u2 := 1; w := 0;
   u3:= -2 \times r/(x+sqrt(x\times(x+4\times r)));
        r := r-1, r-1 while r > 0
   for
                                          dо
   begin
            if large x then
      begin w:= w+mr \times u2; mr:= mr \times (r+1)/(c+r)
      u1:= (-x \times u3 + (v+r) \times u2)/(a+r); u3:= u3-u2; u2:= u1;
```

```
if r > n and r < kmax then u[r-n] := u2;
          r=kmax then uprime:= u3
   end;
   u1:= -x \times u3 + v \times u2; u3:= u3 - u2; v:= a; k:= n-1;
   if kmax=0 then
                     uprime:= u3; kmax:= kmax-n;
   w := if large x then x+(-a)/(a\times(w+c\times u^2)+u^2) else
       x + (-b)/(u1 \times m1 - u3 \times m0);
        r := 0 step 1 until k do v := v/(a+r);
   if n=0 then begin k:=1; u[0]:=w\times u1 end else k:=0;
   w:= vxw; uprime:= wxuprime;
   for r:=k step 1 until kmax do u[r]:=w\times u[r]
end chu;
       procedure uabx(a, b, x, eps, uprime); value
                                                       a, b, x, eps;
real a, b, x, eps, uprime;
begin
       real al, c, p, q, r; integer j, n; array u[0:0];
           a < 0 then
       if
                         entier(a) else 0; q := a1 := a-n; u[0] := 1;
   if n<0 and a=b then
          if a1>0 then chu(a1,a1,x,0,eps,u,q);
   begin
      p := u[0]; r := p-q;
      for j:=1 step 1 until -n do
      begin r := x \times r; q := (al-j) \times p; p := r-q
   end else
   begin if al > 0 then chu(al,b,x,0,eps,u,q);
      c := 1+a1-b+x; al := al-1; p := u[0];
      for j:=1 step 1 until -n do
      begin r := (c-j) \times p - x \times q; q := (al-j) \times (q-p); p := r end;
   end; uabx:= p; uprime:= q
end uabx;
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