

2q+2. Romberg integration is normally given as the extrapolation to the limit of the trapezoid rule. Let

$$T_0^{(k)} = h \left(\frac{1}{2} f_0 + f_1 + \dots + f_{2^{k-1}} + \frac{1}{2} f_{2^k} \right), \text{ and } T_m^{(k)} = \frac{4^m T_{m-1}^{(k+1)} - T_{m-1}^{(k)}}{4^m - 1},$$

then the Romberg quadrature rule gives

$$\int_{t_0}^{t_n} f(t) dt = T_m^{(k)} \approx \sum_{j=0}^n w_j f(t_j),$$

where $n = 2^q$, $m = (p - 2)/2$, and $k = q - m$. The left and right endpoints must be in $t[0]$ and $t[n]$ respectively. The abscissas are returned in $t[0]$ to $t[n]$ and the corresponding weights in $w[0]$ to $w[n]$.

If $p = 2$ the Romberg rule is the same as the repeated trapezoid rule, and if $p = 4$, the same as the repeated Simpson rule.

For $n \leq 128$ and $p \leq 16$, the numerical integration of powers (less than p) of x on the interval $[0, 1]$ gave answers correct to one round off error in an 11-digit mantissa.

REFERENCE: Bauer, F. L., Rutishauser, H., and Stiefel, E. New aspects in numerical quadrature. *Proc. of Symp. in Appl. Math.*, Vol. 15: High speed computing and experimental arithmetic. Amer. Math. Soc., Providence, R. I., 1963, pp. 199-218;

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begin integer i, j, m, m1, m4, s;
real h, ci; real array c[0: (p - 2)/2];
h := (t[n] - t[0])/n; w[0] := w[n] := 0;
for i := n - 1 step -1 until 1 do
  begin w[i] := c[i] := 0; t[i] := i × h + t[0] end;
m := (p - 2)/2; c[0] := 1.0; s := m4 := 1; c[n] := 0;
if m > ln(n)/ln(2) then m := ln(n)/ln(2);
for j := 1 step 1 until m do
  begin m4 := 4 × m4; m1 := m4 - 1;
  for i := j step -1 until 1 do
    c[i] := (m4 × c[i] - c[i - 1])/m1;
  c[0] := c[0] × (m4/m1);
  end;
for i := 0 step 1 until m do
  begin ci := c[i] × s;
  for j := 0 step s until n do w[j] := w[j] + ci;
  s := 2 × s;
  end;
w[0] := w[n] := 0.5 × w[0];
for j := 0 step 1 until n do w[j] := w[j] × h;
end rombergrule

```

ALGORITHM 282

DERIVATIVES OF e^x/x , $\cos(x)/x$, AND $\sin(x)/x^*$ [S22]

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procedure dsubn(x, nmax, d);
value x, nmax; integer nmax; real x; array d;
comment This procedure generates the derivatives

```

$$d_n(x) = \frac{d^n}{dx^n} \left(\frac{e^x}{x} \right) \quad (n = 0, 1, 2, \dots, nmax)$$

using the recurrence relation

$$d_n(x) = (e^x - n d_{n-1}(x))/x \quad (n = 1, 2, 3, \dots).$$

The results are stored in the array d . If $x = 0$, there is an error

exit to a global label called *alarm*;

```

begin integer n; real e;
if x = 0 then go to alarm;
e := exp(x); d[0] := e/x;
for n := 1 step 1 until nmax do
  d[n] := (e - n × d[n - 1])/x;
end dsubn;
procedure csubn(x, nmax, c);
value x, nmax; integer nmax; real x; array c;
comment This procedure obtains the derivatives

```

$$c_n(x) = \frac{d^n}{dx^n} \left(\frac{\cos x}{x} \right) \quad (n = 0, 1, 2, \dots, nmax)$$

from the recurrence relation

$$c_n(x) = (\tau_n(x) - n c_{n-1}(x))/x \quad (n = 1, 2, 3, \dots),$$

where $\{\tau_n(x)\}_{n=1}^{\infty} = \{-\sin x, -\cos x, \sin x, \cos x, -\sin x, \dots\}$.

The results are stored in the array c . If $x = 0$, there is an error exit to a global label called *alarm*;

```

begin integer n; array tau[1: 4];
if x = 0 then go to alarm;
tau[1] := -sin(x); tau[2] := -cos(x);
tau[3] := -tau[1]; tau[4] := -tau[2];
c[0] := tau[4]/x;
for n := 1 step 1 until nmax do
  c[n] := (tau[n - 4] × ((n - 1) ÷ 4) - n × c[n - 1])/x;
end csubn;
procedure ssubn(x, nmax, d, s);
value x, nmax, d; integer nmax, d; real x; array s;
comment This procedure generates to  $d$  significant digits the
derivatives

```

$$s_n(x) = \frac{d^n}{dx^n} \left(\frac{\sin x}{x} \right) \quad (n = 0, 1, 2, \dots, nmax),$$

and stores the results in the array s . The method of computation is based on the recurrence relation

$$s_n(x) = (\sigma_n(x) - n s_{n-1}(x))/x \quad (n = 1, 2, 3, \dots),$$

where $\{\sigma_n(x)\}_{n=1}^{\infty} = \{\cos x, -\sin x, -\cos x, \sin x, \cos x, \dots\}$. The recurrence relation is applied in forward direction as long as $n \leq |x|$, and in backward direction for the remaining values of n , starting with an appropriately large $n = \nu$. A detailed discussion of the method will be published elsewhere. It is assumed that a global real procedure $t(y)$ is available, which evaluates the inverse function $t = t(y)$ of $y = t \ln t$ to low accuracy for $y \geq 0$. (See W. Gautschi, Algorithm 236, Bessel functions of the first kind, *Comm. ACM* 7 (Aug. 1964), 479 Gautschi, W. Computation of successive derivatives of $f(z)/z$, in press;

```

begin integer n, n0, nu; real x1, d1, s1; array sigma [1: 4];
x1 := abs(x);
sigma [1] := cos(x); sigma [2] := -sin(x);
sigma [3] := -sigma [1]; sigma [4] := -sigma [2];
n0 := entier (x1); s[0] := if x ≠ 0 then sigma [4]/x else 1;
for n := 1 step 1 until if n0 ≤ nmax then n0 else nmax do
  s[n] := (sigma [n - 4] × ((n - 1) ÷ 4) - n × s[n - 1])/x;
if n0 < nmax then
  begin
  s1 := 0; d1 := 2.3026 × d + .6931;
  nu := if nmax ≤ 2.7183 × x1 0 then
    1 + entier (2.7183 × x1 × t(.36788 × d1/x1)) else
    1 + entier (nmax × t(d1/nmax));
  for n := nu step -1 until n0 + 2 do
    begin
    s1 := (sigma [n - 4] × ((n - 1) ÷ 4) - x × s1)/n;
    if n ≤ nmax + 1 then s[n - 1] := s1;
    end
  end
  end ssubn

```

ALGORITHM 283

SIMULTANEOUS DISPLACEMENT OF POLYNOMIAL ROOTS IF REAL AND SIMPLE [C2]

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procedure *Prrs* (*A*, *X*, *n*, *eps*); **value** *n*, *eps*;
integer *n*; **real** *eps*; **array** *A*, *X*;
comment *Prrs* (polynomial roots real simple) computes the *n* roots *X* of the polynomial equation

$$A_n x^n + A_{n-1} x^{n-1} + \dots + A_0 = 0$$

simultaneously. On entry the array *X* contains the vector of initial approximations to the roots and on exit it contains the vector of improved approximations to the roots. The initial approximations must be distinct. Accuracy is specified by means of a parameter *eps*. Iteration is continued until the Euclidean norm of the correction vector does not exceed *eps*. The convergence is quadratic;

begin integer *i*, *k*; **real** *x*, *P*, *Q*;
eps := *eps* ↑ 2;
W: *Q* := 0;
for *i* := 1 **step** 1 **until** *n* **do**
begin *x* := *P* := *A*[*n*];
for *k* := 1 **step** 1 **until** *n* **do**
begin *x* := *x* × *X*[*i*] + *A*[*n* - *k*];
if *k* ≠ *i* **then** *P* := *P* × (*X*[*i*] - *X*[*k*])
end;
X[*i*] := *X*[*i*] - *x*/*P*;
Q := *Q* + (*x*/*P*) ↑ 2
end;
if *Q* > *eps* **then go to** *W*
end

CERTIFICATION OF ALGORITHM 9 [D2]

RUNGE-KUTTA INTEGRATION [P. Naur et al.,
Comm. ACM 3 (May 1960), 318]

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Algorithm 9 was transcribed into the hardware representation for CDC 3600 ALGOL and run successfully. The following procedure was used for the global procedure *comp*:

real procedure *comp* (*a*, *b*, *c*); **value** *a*, *b*, *c*; **real** *a*, *b*, *c*;
begin integer *AE*, *BE*, *CE*;
integer procedure *expon* (*x*); **real** *x*;
comment This function produces the base 10 exponent of *x*;
expon := **if** *x* = 0 **then** -999 **else**
entier (.4342944819 × *ln*(*abs*(*x*)) + 1);
comment The number -999 may be replaced by any number less than the exponent of the smallest positive number handled by the particular machine used, for this algorithm assumes that true zero has an exponent smaller than any nonzero floating-point number. Users implementing **real procedure** *comp* by machine code should make sure that this condition is satisfied by their program;

AE := *expon*(*a*); *BE* := *expon*(*b*); *CE* := *expon*(*c*);
if *AE* < *BE* **then** *AE* := *BE*; **if** *AE* < *CE* **then** *AE* := *CE*;
comp := *abs*(*a* - *b*)/10 ↑ *AE*
end

This has the advantage of machine independence, but is highly inefficient compared to machine code.

The procedure was tested using the two following procedures for *FKT*:

procedure *FKT* (*X*, *Y*, *N*, *Z*); **real** *X*; **integer** *N*; **array** *Y*, *Z*;
comment (*dy*₁/*dx*) = *z*₁ = *y*₂, (*dy*₂/*dx*) = *z*₂ = -*y*₁. With *y*₁(0) = 0, *y*₂(0) = 1, the solution is *y*₁ = *sin* *x*, *y*₂ = *cos* *x*;
begin *Z* [*1*] := *Y* [*2*]; *Z* [*2*] := -*Y* [*1*] **end**;
procedure *FKT* (*X*, *Y*, *N*, *Z*); **real** *X*; **integer** *N*; **array** *Y*, *Z*;
comment (*dy*₁/*dx*) = 1 + *y*₁². For *y*₁(0) = 0, *y*(*x*) = *tan* *x*;
Z [*1*] := 1 + *Y* [*1*] ↑ 2;

The *RK* procedure was used to integrate the differential equations represented by the first *FKT* procedure from *x* = 0(0.5)7.0, with *eps* = *eta* = 10⁻⁸, and with *y*₁(0) = 0, *y*₂(0) = 1. The actual step size *h* was .0625 for most of the range, but was reduced to .03125 in the neighborhood of *x* = *k*π/2, where one or the other of the solutions is small.

The computed solutions at *x* = 7.0 were: *y*₁ = 6.5698602746 × 10⁻¹, *y*₂ = 7.5390270246 × 10⁻¹, with errors -5.71 × 10⁻⁷ and 4.48 × 10⁻⁷, respectively.

Results for the second differential equation are summarized in Table I below.

The efficiency of the procedure would be increased slightly on most computers by changing the type of the **own** variables from **real** to **integer**.

The error is estimated by comparing the results of successive pairs of steps with that of a single double step. This is somewhat more time-consuming than the Kutta-Merson process presented in Algorithm 218 [*Comm. ACM* 6 (Dec. 1963) 737-8]. However, the criterion for step-size variation in Algorithm 9 which effectively applies an approximate relative error criterion, *eps*, for |*y*| > *eta*, and an absolute error criterion *eta* × *eps*, for |*y*| < *eta*, appears superior when the solution fluctuates in magnitude.

REMARK ON ALGORITHM 218 [D2]

KUTTA-MERSON [Phyllis M. Lukehart, *Comm. ACM* 6 (Dec. 1963), 737]

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Successive calls of *Kutta Merson* with *first* = **false** do not reach the upper bound *t*+*h* if the interval *h* is unequal to the interval *h* of the first call with *first* = **true**.

Proposed correction:

- 1) declaration **real** *hc*, instead of **own real** *hc*;
- 2) **if** *first* **then begin** **for** *i* := 1 **step** 1 **until** *n* **do** *y*₀[*i*] := *y*[*i*];
hc := *h*; *ploc* := 1; *first* := **false**
end else *hc* := *h*/*ploc*;
instead of **if** *first* **then begin** ... **end**;

TABLE I [ALG. 9]

	η	x = 0.5			x = 1.0			x = 1.5		
		<i>h</i> _{min}	Absolute error	Relative error	<i>h</i> _{min}	Absolute error	Relative error	<i>h</i> _{min}	Absolute error	Relative error
10 ⁻⁷	10 ⁻³	.03125	-1 × 10 ⁻⁹	-2 × 10 ⁻⁹	.03125	9 × 10 ⁻⁸	6 × 10 ⁻⁸	.00390625	-1 × 10 ⁻⁶	-8 × 10 ⁻⁸
10 ⁻⁵	10 ⁻³	.125	-5 × 10 ⁻⁷	-9 × 10 ⁻⁷	.0625	8 × 10 ⁻⁷	5 × 10 ⁻⁷	.0078125	-2 × 10 ⁻⁴	-1 × 10 ⁻⁵
10 ⁻³	10 ⁻³	.25	-1 × 10 ⁻⁵	-2 × 10 ⁻⁵	.25	-2 × 10 ⁻⁴	-1 × 10 ⁻⁴	.03125	-3 × 10 ⁻²	-2 × 10 ⁻³