The data for an evaluation are the numerical values of the orbital parameters A, α , etc. The first stage of the calculation is the evaluation of all the auxiliary functions, it not being thought worthwhile to program the selection only of those required for the particular integral. Similarly no attempt was made to carry over the values of any of the auxiliary functions from one integral to another.

The successive terms of the multinomial were then evaluated and their sum accumulated. At this stage a check on the accuracy of the evaluation was carried out. All arithmetic was in the floating-point mode with a binary exponent and a nominal precision of 38 significant binary digits. The maximum exponent over all terms and over all partial sums was recorded. The excess of this over the exponent of the final result is a measure of the differencing error incurred. Numerous evaluations have suggested that this error does not amount to more than two or three binary digits.

In the evaluation of each term $C \prod x_{i}^{u}$ the array u was

scanned and zero entries ignored. The remaining factors were formed by using the digits of the binary representation of $mod(u_i)$ to select contributions from the sequence obtained by repeatedly squaring x_i or $1/x_i$. Each term was evaluated independently of the rest. Were it not for the limited rapid-access storage available on the machines used, it might have been worthwhile preserving some information from one term to the next. Thus the sequence x_j , x_j^2 , x_j^4 , ... might have been preserved. For $u_j > 0$, $x_j^{u_j}$ would have been calculated as a product of selections from this sequence as before;

for $u_i < 0$ then $1/x_i^{-u_j}$ would have been calculated. The terms of the sequence would best be calculated when first required; the number of terms currently available could be stored and the sequence could readily be extended as needed.

It is thought that the speed of evaluation could be significantly increased on suitable machines in this way. There are, however, further improvements which are theoretically possible and which would be very rewarding if means could be devised for implementing them automatically. The simplest example is the insertion of brackets in the expression for a polynomial prior to evaluating it by nested multiplication thus:

$$ax^{3} + bx^{2} + cx + d = ((ax + b)x + c)x + d.$$

Still more efficient means of evaluating polynomials are discussed by Knuth (1962). The present paper shows how general functions of several variables may be reduced to multinomials, albeit with some loss of efficiency due to unexploited dependency among the auxiliary functions. Even in this limited field, however, there appears to be no theoretical treatment of the evaluation problem. Any proposal, to be useful in the present context, must be capable of evaluating efficiently an expression whose precise form is not known to the programmer. This is, of course, a much greater problem than that posed by the evaluation of any particular expression, however complex.

One of the authors (R.F.) is indebted to the Department of Scientific and Industrial Research for the provision of a Research Studentship.

7. References

Boys, S. F. (1950). "Electronic Wavefunctions I," Proc. Roy. Soc. London, Vol. A200, p. 542.

BOYS, S. F., and COOK, G. B. (1960). "Mathematical Problems in the Complete Quantum Prediction of Chemical Phenomena." Rev. Mod. Phys., Vol. 32, p. 285.

COOPER, D. C. (1961). Formal Differentiation of Algebraic Expressions: An Example in List Processing. University of London Computer Unit Internal Memorandum.

HANSON, J. W., CAVINESS, J. S., and JOSEPH, C. (1962). "Analytic Differentiation by Computer," Comm. A.C.M., Vol. 5, p. 349.

KNUTH, D. E. (1962). "Evaluation of Polynomials by Computer," Comm. A.C.M., Vol. 5, p. 595.
MCCARTHY, J. (1960). "Recursive Functions of Symbolic Expressions and their Computation by Machine, Part I," Comm. A.C.M., Vol. 3, p. 184.

NOTICE TO MEMBERS OF THE BRITISH COMPUTER SOCIETY

Overseas Society Publications

Members, Associate Members, and Students of the British Computer Society resident in the British Isles are reminded that they may subscribe at reduced prices to the publications of certain overseas computer societies, affiliated to I.F.I.P. Details may be obtained from the Assistant Secretary, at the address given on p. ii of the cover.

The Association for Computing Machinery announces that the special price at which B.C.S. members resident in the British Isles may subscribe inclusively to A.C.M. Journal, Communications, and Computing Reviews will be increased with effect from 1 January 1964 to £5 0s. 0d. (\$14.00); A.C.M. membership fees will then be \$18.00 and the normal subscription price for non-members to each of the A.C.M. publications will be increased to \$15.00 on that date.

B.C.S. members and others should remit subscriptions to the Assistant Secretary, quoting their membership number where applicable.