Computers chem. Engng, Vol. 15, No. 12, p. 859, 1991
Printed in Great Britain

0098-1354/91 $3.00 + 0.00
Pergamon Press plc

LETTER TO THE EDITORS

We would like to thank Dr Michelsen and Dr Villadsen for their interest in our papers (Quan and Chang, 1989ab) and their constructive comments given in a recent *Letter to the Editors* (Michelsen and Villadsen, 1991). Although we agree with some of their opinions, it is still our belief that our approach possesses a number of unique features which are quite desirable in solving nonlinear differential equations.

First, let us examine the time required for computing the quadrature coefficients using various different techniques. Numerical experiments have been carried out on a 286 PC using TURBO PASCAL. The results corresponding to 3–25 grid points are summarized in Fig. 1. The curve labelled by "recursive" represents the elapsed time on a PC using the recursive procedure published by Villadsen and Michelsen (1978). The other curves are the results obtained by implementing the procedure proposed by Quan and Chang (1989a). The one marked by "$P_n^{(r,s)}(x)$" indicates that the grid points are located at the zeros of a Jacobi polynomial. The symbol "$L^{(r)}(x)$" denotes that the zeros of a Laguerre polynomial are used. From Fig. 1, one can see that two of the most efficient schemes are corresponding to the Chebyshev polynomials of the first and second kind, i.e. $T_n(x)$ and $U_n(x)$. Notice that they are special cases of the Jacobi polynomials. In recent studies (Chang and Quan, 1989; Lin, 1991), we have found that in the case of Chebyshev polynomials, further simplifications to the "simplified formulas" presented in Quan and Chang (1989a) are possible and, thus, the time needed for calculating the quadrature coefficients reduces to about 1/6 of that of the recursive algorithm. In addition, explicit formulas of the quadrature coefficients are presented for arbitrarily-distributed grid points in Quan and Chang [(1989a), equations (18–21)]. These formulas are as general as the recursive algorithm and the computing time is about the same. They were thus not used in most of our application examples (Quan and Chang, 1989b) due to their inefficiency. However, these equations are still useful in developing additional simplification techniques for symmetrical systems (Quan and Chang, 1989a). On the other hand, the same simplifications cannot be achieved directly from the recursive formulas suggested by Villadsen and Michelsen (1978).

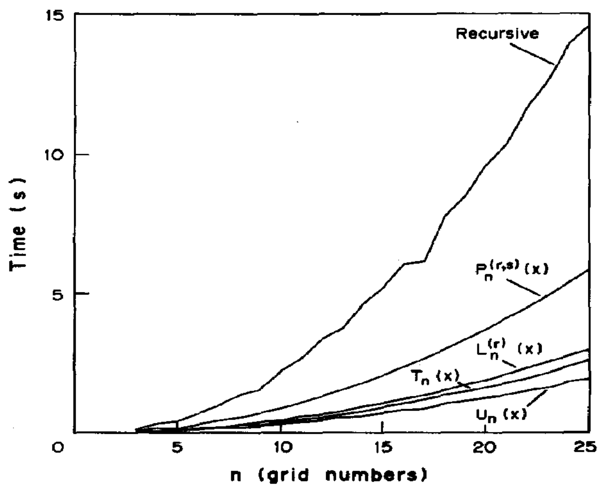

Fig. 1

One of the disadvantages of the Method of Weighted Residuals (and the Method of Differential Quadrature) is that the accuracy of the approximate solution is difficult to determine in advance (Finlayson, 1980, p. 65). Thus, a common practice to ensure the accuracy of results is to gradually increase the number of grid points until the numerical answers do not change appreciably. In such cases, the use of our approach is especially convenient and time-saving. Further, based on the results of a limited number of examples we have studied so far, the accuracy achieved by using the zeros of the Chebyshev polynomials as the grid points is in general very close to "optimal". This is in fact demonstrated in the *Letter to the Editors* by Michelsen and Villadsen (1991). The average relative errors of the two different methods are of the same order of magnitude. It is our opinion that, when comparing different grid point placement schemes, not only the accuracy in numerical solutions but also the ease and efficiency of implementation must be considered. Thus, we conclude that there are enough incentives for selecting our approach for solving nonlinear differential equations.

Finally, we would like to point out that we *did* mention the recursive algorithm in our previous paper (Quan and Chang, 1989a, p. 782). Since our study was initiated from an analysis of the Method of Differential Quadrature, the "conventional" approach for computing the quadrature coefficients is thus the inversion of the Vandermonde matrix which has been used in all the related publications available to us.

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REFERENCES

Chang C. T. and J. R. Quan, A unified approach for solving nonlinear differential equations in process models. *IChemE Symp. Ser.* **114,** 177 (1989).

Finlayson B. A., *Nonlinear Analysis in Chemical Engineering*. McGraw-Hill, New York (1980).

Lin T. T., Application of a generalized quadrature method in solving boundary-value problems. M. S. Thesis, National Cheng Kung University, Tainan, Taiwan (1991).

Michelsen M. L. and J. V. Villadsen, Letter to the Editor. *Computers chem. Engng* **15,** 145 (1991).

Quan J. R. and C. T. Chang, New insights in solving distributed system equations by the quadrature method —I. Analysis. *Computers chem. Engng* **13,** 779–788 (1989a).

Quan J. R. and C. T. Chang, New insights in solving distributed system equations by the quadrature method—II. Numerical experiments. *Computers chem. Engng* **13,** 1017–1024 (1989b).

Villadsen J. V. and M. L. Michelsen, *Solution of Differential Equation Models by Polynomial Approximation*. Prentice-Hall, Englewood Cliffs, NJ (1978).