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This Week's Citation Classic

Villadsen J V & Stewart W E. Solution of boundary-value problems by orthogonal collocation. *Chem. Eng. Sci,* 22:1483-501, 1967. [Department of Chemical Engineering, University of Wisconsin, Madison, WI]

A standard method for treatment of differential equation models was discovered more or less by chance when applying a quadrature-Galerkin method to solve a simple chemical engineering problem. The method was easy to use and it made manual solution of even complicated problems seem possible. [The *SCI*® indicates that this paper has been cited over 165 times since 1967.]

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"Fortunate circumstances combined to make this paper possible. When I went to Wisconsin in 1965 on a NATO Senior Research Fellowship, Warren Stewart was interested in weighted residual methods (MWR) and I had just 'discovered' numerical quadratures in Kopal's classical text[1] and wanted to apply them to chemical engineering problems.

"The idea was to solve differential equations by MWR and to evaluate the integrals which appear in these methods by optimal numerical quadrature. First, we treated linear effectiveness factor problems and here the N integrals of 'residual multiplied by trial functions' which appear in Galerkin's method —one of the most powerful MWR —would all be zero if the residual was proportional to a Jacobi polynomial. Hence, if the residual was zero at the N zeros of the appropriate polynomial, N algebraic equations in the coefficients of the Nth order polynomial approximation for the solution were immediately obtained by quadrature. This was a collocation method and since the quadrature used zeros of an orthogonal polynomial (a Jacobi polynomial) the method was called orthogonal collocation. Now, the Galerkin method was highly respected while collocation methods, although easy to apply, were known to be unsafe. Thus, the copying of Calerkin's method by one particular collocation method seemed to be a major step forward.

"Looking back on the paper from a distance of 15 years, two aspects seem to be noteworthy. very primitive formulas were used to discretize derivatives and even the construction of the polynomials was difficult. There is a good reason why the highest approximation used in the paper (tables 2 to 4) is N = 3: the polynomials were manually constructed by complicated procedures and it seemed impossible to handle the work beyond N = 3. A modern text on numerical methods in chemical engineering such as *Solution of Differential Equation Models by Polynomial Approximation*[2] treats the subject much more relaxed. Students apply computer programs to set up any collocation scheme of arbitrary order and proceed directly to solve all sorts of problems.

"Still, the original paper with its cumbersome mathematics had one nice feature: the examples were easy to follow and practically all subjects which **were** later treated successfully by collocation were described—boundary value problems, eigenvalue problems, and parabolic and elliptic partial differential equations.

"This, in my opinion, was a major reason for the rapid acceptance of orthogonal collocation as a standard method for solution of differential equation models. The paper appeared at a time when a lot of people were studying these models, it offered an easy, mechanical way of handling MWR on computers, and the accuracy was impressive compared to finite difference methods. Later studies by ourselves and by others have clarified the mathematical background and within each of the subjects treated by the original paper much more difficult problems have been solved."

1. **Kopal** Z. *Numerical analysis.* New York: Wiley, 1955. 556 p.
2. **Villadsen J & Michelsen M L.** *Solution of differential equation models by polynomial approximation.* Englewood Cliffs, NJ: Prentice .Hall, 1978. 446 p.