Preface to the Classics Edition

This book was originally published in 1972, when computers were just beginning to make an impact on the solution of differential equations. The first part of it treats differential equations governing transport problems of flow, heat, and mass, using approximate methods and a series of functions but only a few terms. The second part describes variational principles (or not) for those problems and uses variational principles to derive error bounds that can be calculated for some problems. This was important because the series used in the approximate methods for nonlinear problems could not be extended to a large number of terms without the use of a computer. Since then computers have advanced considerably and much more sophisticated numerical techniques are available, but the mathematical principles described herein are still valid and still useful. Thus, I am very pleased to have it included in the SIAM Classics series. Areas such as optimization, spectral methods, and error bounds using mesh refinement have advanced considerably, and suggestions for current information are given below.

In my own historical journey, in 1972 it was important to have simple approximate solutions that could be calculated easily to show the basic behavior of the solutions to differential equations using reduced models. The Galerkin, collocation, least squares, and integral methods were all subsumed under the phrase *method of weighted residuals* [5]. But the approximate nature of the solution made it important to test the solutions with mathematically rigorous error bounds. Several of my graduate students did this in their theses, and their results are included in the book. At the time, I used the term *variational methods* exclusively for problems with a functional that was to be made stationary or an extremum, and chapters in the book show how to find such a function, if it exists. But, in the intervening time, the term variational has been applied to any method that makes the residual orthogonal to a set of complete functions, whether a stationary variational principle exists or not. At the time the book was written, the finite element method had been developed extensively in civil engineering for structural problems, especially linear ones (which usually had variational principles), and it was just beginning to be used to solve differential equations arising in heat transfer and fluid mechanics. Thus, the treatment here of the finite element method is elementary and concise but clear. An important point is the role of natural boundary conditions, since they are derived from a variational principle. Currently, it is clear to the author that some people who apply the finite element method don't understand the relation between the natural boundary condition and the variational principle. Thus, they expect a natural boundary condition to be satisfied exactly, when its role is really to integrate the impact of the surroundings on the solution domain. The treatment of variational principles here explores that topic mathematically. In addition, the adjoint variational problem is introduced for almost any nonlinear problem, and this sometimes helps in establishing error bounds for an approximate solution. The last chapter provides a number of theorems on error bounds. The error bound is often found in terms of the residual, which is the differential equation with the approximate solution inserted. Those theorems are still valid and can be used in modern computer packages to provide rigorous error bounds. Many other theorems are available now, of course (see the books listed below), but often only for linear problems.

My 1980 book, "Nonlinear Analysis in Chemical Engineering" [7], is heavily oriented towards numerical methods that can be applied to nonlinear problems. Yet it builds on the first one by expanding the treatment of the orthogonal collocation method that was being used widely within chemical engineering. Outside of chemical engineering, the polynomials are called Chebyshev, Legendre, or Jacobi polynomials, and spectral methods are used, as referenced below. The 1980 book also introduced the ideas for integration in time of stiff differential equations, as developed primarily by Gear [11], that made it possible to solve complicated nonlinear problems without spending great effort figuring out what time step size would be suitable. The finite element method was now in full application to fluid flow, heat transfer, and mass transfer, so that these methods were expanded greatly. But errors were assessed not by mathematical error bounds but by doing mesh refinement and seeing whether the solution was affected. Of course, there weren't error bounds for all problems, but the material in Chapter 11 here is still valid and can still be applied. Some finite element software, such as Comsol Multiphysics (see [9]), does allow the user to calculate the residual after a solution is found and has an option for mesh refinement using an estimate of the global error.

My 1992 book, "Numerical Methods for Problems with Moving Fronts" [8], treated numerical methods for problems with steep gradients that are moving, which is one type of problem not in the "Nonlinear Analysis" book. In some applications, the approximate methods in this book can be combined analytically with the numerical solution to ease the numerical problem of high convection.

My 2006 book, "Introduction to Chemical Engineering Computing" [9], was written with the realization that many differential equations are solved today by packages written by others. The user's role then is to validate the solution rather than program the computer to solve the problem. Details can be left to websites, such as the author's description of the numerical methods in

http://faculty.washington.edu/finlayso/ebook.

In addition, hp-methods involve reducing the mesh size (h) and increasing the degree of the polynomials (p) [3].

Today, solution on different meshes, each more refined than the last, are often the only guide to the error in the solution. Here again, though, packages like Comsol Multiphysics (see [9]) are useful because they make it possible to easily calculate the residual, and it is possible to see the residual decrease as the approximation improves. If one of the theorems in Chapter 11 holds, the error bound is established. The website www.ChemEComp.com has additional information about the Introduction to Chemical Engineering book. Since error bounds are important (and often neglected), some new problems derived from Chapter 11 of this Classics edition are available from SIAM (www.siam.org/books.cl73) and www.ChemEComp.com/MWR. Some problems have solutions, and some do not. Instructors may ask SIAM (textbooks@siam.org) for the key to the problems without a key.

Optimization is not discussed in the 1972 book, but the orthogonal collocation method led to a fast method for dynamic optimization, as described by Biegler [1]. The speed-up resulted because the solution was expanded in terms of orthogonal polynomials but the collocation equations didn't need to be solved at each step in the optimization, using successive quadratic programming. The number of iterations was sometimes less than 5% of a standard method. Later, Biegler [2] reviewed simultaneous strategies for dynamic optimization in which the state and control profiles in time are discretized using collocation on finite elements. While this leads to large-scale nonlinear program problems, efficient strategies to solve them have been found. They are now called the direct transcription method or the simultaneous collocation method [20]. Applications include collision avoidance for aircraft and trajectories for satellites, among others [2]. These references are cited because the work on orthogonal collocation in the 1972 and 1980 books led to an important part of the algorithm. In addition, SIAM has published a variety of books on optimization [4, 6, 13, 14, 17, 18].

Another area that has advanced considerably since this book was written is in spectral methods. Lanczos [15, 16] is referred to for Chebyshev (orthogonal) polynomials, which basically became know as the orthogonal collocation method in chemical engineering. But Chevyshev polynomials have been used extensively and connect with Fourier spectral methods for solving differential equations. See especially “Chebyshev Polynomials in Numerical Analysis” [10] by Fox and Parker, “Numerical Analysis of Spectral Methods” [12] by Gottlieb and Orszag (including advection problems and mesh refinement), “Spectral Methods in MATLAB” [21] by Trefethen, “Spectral Methods: Evolution to Complex Geometries and Application to Fluid Dynamics” [3] by Canuto et al., and “Chebyshev Polynomials” by Mason and Handscomb [19] (including error analysis).

While the main thrust of modern computing seems to be to solve the entire problem in all its detail using the computer, sometimes part of the solution are essentially known, such as what happens in a thin region with heat transfer perpendicular to the thin region; it is really unnecessary to use a finite element mesh inside the thin region for certain parameters. Then it is possible to use the simple, approximate methods described below in conjunction with the computer programs, leading to a less complex model which includes more understanding of the problem. Paraphrasing Einstein, make the model as complicated as needed, but no more complicated. As a simple example, shown here and in my later books, for many problems a small time solution can be obtained analytically, and this can be combined with the full numerical problem to provide a solution which is accurate at all times and does not oscillate at small times; frequently the finite difference method and finite element method, by themselves, oscillate from node to node in the first few time steps, and the analytical approximations described here can be used to define a problem without this difficulty.

I encourage modern readers to use the full knowledge of mathematics to validate the best solution possible, and I hope this SIAM Classics book will contribute to that progress. The book was a highlight of my early career, and I've been thankful that Academic Press originally published it. Now is has been wonderful to work with the staff at SIAM as this book was being produced for this Classics edition.

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