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Edited by C. A. Brebbia and S. A. Orszag

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W. J. Lick

Difference Equations from Differential Equations

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PREFACE

In computational mechanics, the first and quite often the most difficult part of a problem is the correct formulation of the problem. This is usually done in terms of differential equations. Once this formulation is accomplished, the translation of the governing differential equations into accurate, stable, and physically realistic difference equations can be a formidable task. By comparison, the numerical evaluation of these difference equations in order to obtain a solution is usually much simpler. The present notes are primarily concerned with the second task, that of deriving accurate, stable, and physically realistic difference equations from the governing differential equations. Procedures for the numerical evaluation of these difference equations are also presented. In later applications, the physical formulation of the problem and the properties of the numerical solution, especially as they are related to the numerical approximations inherent in the solution, are discussed.

There are numerous ways to form difference equations from differential equations. Some are more successful than others with the success of any particular method quite often dependent on the problem to be solved. The first widely used method was the finite difference method. In this method, one obtains difference equations by the use of local expansions for the variables, generally truncated Taylor series. This procedure is relatively simple and has been extensively used in practically all areas of dynamics where numerical approximations have been needed. As with any approximate method, the procedure has its shortcomings, e.g., frequent instability of the derived difference equations and difficulty in properly treating boundary conditions.

In order to better derive the appropriate difference equations and eliminate some of these difficulties, a volume integral method was developed (Tikhanov and Samarskii, 1956; Varga, 1962). In this method, the region of interest (in space and time) is divided into finite volume elements. The governing equations are then integrated over each of these elements. In order to form a difference equation, the terms in the resulting equations must then be analytically approximated as well as possible. Various approaches to do this have been developed; the most conventional and widely used procedure is to approximate these terms using Taylor series expansions. This procedure as well as improvements to this procedure will be described here. The volume integral method is quite general (e.g., the usual finite-difference equations obtained by means of Taylor series can also be obtained by this method as a special case) and it has been widely used as a natural extension of the finite difference procedure without much recognition of its versatility and power.

More recently, a general class of procedures called finite element methods has been developed. To a large extent, these methods have appealed to engineers and scientists because, just as in the volume integral method, the entire continuum is divided into a series of control volumes or finite elements, each of which has physical meaning. The methods have been extensively applied to problems in continuum dynamics, primarily in structures but also in fluid dynamics.

Finite element methods usually consist of first multiplying the governing equations by a weighting function (which may be a known function or the solution itself) and then integrating the results over a volume element. In order to obtain a difference equation, the solution and the weighting function are usually approximated by polynomials. This approach is especially satisfactory for linear, non-dissipative systems. In this case, the procedure is equivalent to finding the minimum or maximum value of a functional (such as the potential energy of a system) and the solution is then the quantity that minimizes this functional. For these and similar problems, the integrals of the weighted equations have theoretical and physical significance and finite element methods work well. For other cases, this is no longer true and finite element methods have not proved to be as satisfactory. At the present time, finite element methods are quite popular, especially in solid mechanics, for the above reasons and also because (a) the grid points can be arbitrarily placed and problems with irregular boundaries can then be treated more easily, and (b) the accuracy of the approximation can be improved relatively easily by using higher order polynomials.

The finite difference, volume integral, and finite element methods can all be included as special cases of a generalized finite element method (Zienkiewicz and Morgan, 1983). A unified formulation, at least in theory, is then possible to cover all approximation processes. It can also be readily shown that all three methods quite often give identical approximation equations. However, although there are many similarities, the three methods differ significantly in their practical details and are usually formulated independently of each other.

Both the finite difference and finite element methods have significant limitations. The volume integral method is superior to both of these methods in many respects and, in the present notes, will be the primary method used in deriving difference equations. Specific reasons for this choice are as follows. (1) The volume integral method is a logical extension of the finite difference procedure with all its advantages but not all of its disadvantages. Because of this, almost all of the work on finite difference equations is directly applicable to the present method. (2) In the volume integral method, control volumes or finite elements are used and the governing equations are then satisfied on the average over each element. In this sense, the present method is analogous to the finite element method. As in that method, the elements need not be uniform but can be variable in size as well as triangular or another shape. Because of the use of volume elements, the derivation of the correct difference equations at boundaries (closed as well as open) is considerably simplified. (3) The integral method works directly with the fundamental equations, e.g., the conservation equations, rather than with weighted equations as does the usual finite-element method. The use of volume elements along with the governing equations in conservation form allows one to enforce exact conservation of the dependent variables (e.g., mass, momentum, and energy) as an integral over each element and between each element as well as globally. This is not true for some finite difference and for most finite element algorithms.

Other advantages of the integral method follow from an extension of the usual procedure, an extension that incorporates approximate analytic solutions to the differential equation in the formation of the corresponding difference equation. When a good approximation to the differential equation is known, the accuracy of the corresponding difference equation may be greatly increased over that obtained by the standard Taylor series approximations. From this point of view, Taylor series approximations are just comparatively poor solutions of the differential equation and lead to crude difference equations. The use of approximate analytic solutions also allows one to readily transfer the analytic statements which one uses to approximate the physics into numerical algorithms. This is especially useful at boundaries, where the derivation of the correct numerical algorithm is simplified.

It will also be seen that, by using the present approach and making realistic approximations to the solution within an element, it is very difficult to derive an incorrect algorithm, that is, one that is inaccurate, completely unstable, or not reflecting the proper physics. Although not completely foolproof, the procedure is almost foolproof and is relatively unambiguous.

In Chapter 1, the volume integral method is applied to ordinary differential equations. The purpose is not only to derive accurate, stable, and efficient algorithms for ordinary differential equations but also to develop the proper ideas and procedures for later use in deriving difference equations from partial differential equations.

Basic concepts in the applications of the volume integral method to partial differential equations are discussed in Chapters 2, 3, and 4. Chapter 2 is concerned with parabolic partial differential equations with much of the discussion centered on the simple but important equation governing one-dimensional, time-dependent heat conduction. Other more general parabolic equations are also treated. Chapter 3 is concerned with hyperbolic equations, a representative case being the one-dimensional, time-dependent linear wave equation. Equations for linear wave propagation in two space dimensions as well as nonlinear wave equations are also discussed. In Chapter 4, the derivation of difference equations for elliptic partial differential equations is presented. These equations usually evolve from the steady-state limit of solutions where the time-dependent problem is described by parabolic or hyperbolic equations. Hence, the discussion of elliptic equations after parabolic or hyperbolic equations seems natural, even though in some ways elliptic equations seem simpler than the other two.

Applications of these ideas and algorithms to specific problems are presented in Chapter 5. The purpose here is to demonstrate the use of the basic ideas developed in Chapters 1 through 4 to a variety of problems of practical interest. Specific problems are: lake currents, sediment transport, chemical vapor deposition, and free-surface flows around submerged or floating bodies. In each case, the formulation of the problem, the derivations of the appropriate difference equations, the solution of these equations, and a brief discussion of the results, especially as they are related to the numerical approximations inherent in the solution to the problem, are presented.

The present notes differ from a standard text on numerical analysis in several ways. First, except for introductory material, the only procedure used here to derive difference equations from differential equations is the volume integral method. The derived equations include most of the standard types of finite difference algorithms as well as many others. The use of only one procedure to derive difference equations rather than the use of several procedures as is usually done hopefully makes the presentation easier to understand. The idea is not only to present the difference equations and their derivations but more generally to present a rational procedure for deriving new and improved difference equations.

Second, the derivation and use of the difference equations are related more closely to the basic physical problem than is ordinarily done in a standard text. This is done because it is believed that a good understanding of the correct formulation of the problem and at least a qualitative understanding of the solution to the problem are both useful in the derivation of the optimum difference equation and in obtaining an accurate numerical solution.

It will be seen that the present notes describe mostly elementary theory and applications. Nevertheless, it is hoped that the notes do demonstrate the potential of the volume integral method and, because of this, will encourage further work on this method.

Much of the work presented here was done as part of the author's research on water pollution. As such, the work was partially supported by the U.S. Environmental Protection Agency. Dr. Louis Swaby, Mr. Bill Richardson, and Dr. Anthony Kizlauskas were the project officers. I am grateful to them for their support and encouragement. I would like to thank Dr. C. Kirk Ziegler for many discussions on numerical methods and for doing many of the calculations. James Lick was responsible for much of the graphical work. I am also grateful to Ms. June Finney for her great patience and care in typing and proofreading the manuscript.

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1. ORDINARY DIFFERENTIAL EQUATIONS

The major purpose of the present chapter is to demonstrate the use of the volume integral method in deriving accurate, stable, and physically realistic difference equations from ordinary differential equations. A secondary purpose is to develop the proper ideas and procedures for later use in deriving difference equations from partial differential equations.

Ordinary differential equations come in many different shapes and sizes and can be described, for example, by such terms as (a) a single equation or a system of equations; (b) first-order, second-order, or higher-order equations; (c) linear or nonlinear; and (d) homogeneous or non-homogeneous. These terms describe different properties of ordinary differential equations and certainly the difference equations derived from these differential equations must reflect these properties, at least in some approximate manner. Nevertheless, the general procedure for deriving difference equations by means of the volume integral method does not depend on these properties.

Problems described by ordinary differential equations can also be classified as either initial-value problems or boundary-value problems. In initial-value problems, the solution depends on conditions prescribed only at one end of the interval of interest. In boundary-value problems, the solution depends on conditions prescribed at both ends of the interval. The distinction between initial-value and boundary-value problems is of importance in the application of the volume integral method. It will be seen later that this distinction is also of importance in partial differential equations.

The chapter begins by illustrating the derivation of difference equations from simple differential equations by the conventional approach, by the use of Taylor series. The volume integral method is then introduced and illustrated by applications to the same differential equations. Extensions and more interesting applications of the method to boundary-value problems (second order), initial-value problems (first- or higher-order), and higher-order boundary-value problems are then presented. For simplicity, the assumption is generally made that the grid spacing is uniform; however, for generality, the procedure for deriving difference equations with non-uniform grid spacing is also presented and demonstrated in a few cases.

1.1 Difference Equations by Means of Taylor Series

As a first example, consider one-dimensional, steady-state heat conduction in a solid ($0 \leq x \leq 1$). The solid is assumed to have constant properties. Internal heat sources are present such that the heating is proportional to $-x^{1/2}$. The surface temperature of the solid at x = 0 is kept fixed while the other surface at x = 1 is insulated. In dimensionless variables, the appropriate equations are:

$$\frac{d^2u}{dx^2} = x^{1/2}, \qquad u(0) = 0, \qquad \frac{du}{dx}(1) = 0 \tag{1.1.1}$$

The exact solution to this problem is

$$u = \frac{4}{15}x^{5/2} - \frac{2}{3}x \tag{1.1.2}$$

and is shown in Figure 1.1-1.

Taylor Series (Uniform Grid)

Let us review the standard procedure for obtaining difference equations from differential equations by means of Taylor series. The interval $0 \leq x \leq 1$ is first divided into I-1 equally spaced intervals such that

$$x_i = (i - 1)\,\Delta x, \qquad i=1,2,...,I \tag{1.1.3}$$

The dependent variable u(x) will be evaluated at these grid points and is given there by

$$u(x_i) = u_i \tag{1.1.4}$$

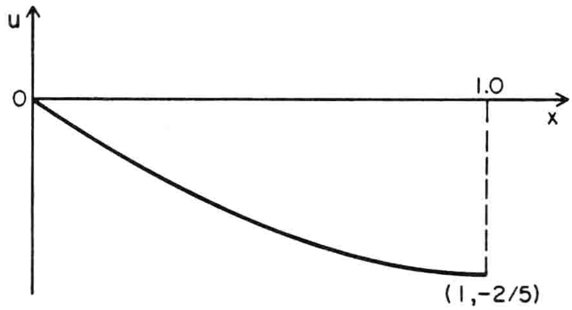

Figure 1.1-1. Plot of $u = \frac{4}{15}x^{5/2} - \frac{2}{3}x$.

By expanding u(x + Δx) in a Taylor series about the point x, one obtains

$$u(x + \Delta x) = u(x) + \frac{du}{dx}(x)\Delta x + \frac{d^2u}{dx^2}(x)\frac{\Delta x^2}{2} + \frac{d^3u}{dx^3}(x)\frac{\Delta x^3}{3!} + \ldots \tag{1.1.5}$$

In the notation defined above, this becomes

$$u_{i+1} = u_i + \left(\frac{du}{dx}\right)_i \Delta x + \left(\frac{d^2u}{dx^2}\right)_i \frac{\Delta x^2}{2} + \left(\frac{d^3u}{dx^3}\right)_i \frac{\Delta x^3}{3!} + \ldots \tag{1.1.6}$$

Similarly, the value of u(x-Δx) can be written as

$$u_{i-1} = u_i - \left(\frac{du}{dx}\right)_i \Delta x + \left(\frac{d^2u}{dx^2}\right)_i \frac{\Delta x^2}{2} - \left(\frac{d^3u}{dx^3}\right)_i \frac{\Delta x^3}{3!} + \ldots \tag{1.1.7}$$

The derivative $(du/dx)_i$ can readily be approximated from the above equations.

From Eq. (1.1.6), one obtains

$$\left(\frac{du}{dx}\right)_i = \frac{u_{i+1} - u_i}{\Delta x} - \left(\frac{d^2u}{dx^2}\right)_i \frac{\Delta x}{2} + \ldots$$

$$= \frac{u_{i+1} - u_i}{\Delta x} + 0(\Delta x) \cong \frac{u_{i+1} - u_i}{\Delta x} \qquad (1.1.8)$$

This is referred to as a forward difference approximation to $(du/dx)_i$ and is accurate up to terms of $0(\Delta x)$, i.e., the truncation error is $0(\Delta x)$. It is a first-order approximation, or a first approximation to $(du/dx)_i$.

Similarly, one can solve Eq. (1.1.7) for $(du/dx)_i$ and one obtains

$$\left(\frac{du}{dx}\right)_i = \frac{u_i - u_{i-1}}{\Delta x} + \left(\frac{d^2u}{dx^2}\right)_i \frac{\Delta x}{2} + \ldots$$

$$= \frac{u_i - u_{i-1}}{\Delta x} + 0(\Delta x) \cong \frac{u_i - u_{i-1}}{\Delta x} \qquad (1.1.9)$$

This is referred to as a backward difference approximation to $(du/dx)_i$. Eqs. (1.1.8) and (1.1.9) are of the same accuracy. Which one is used as an approximation in an equation depends on the problem as will be demonstrated later.

A more accurate expression for $(du/dx)_i$ can be obtained by subtracting Eq. (1.1.7) from Eq. (1.1.6) and solving for $(du/dx)_i$. One obtains

$$\left(\frac{du}{dx}\right)_i = \frac{u_{i+1} - u_{i-1}}{2\Delta x} - \left(\frac{d^3u}{dx^3}\right)_i \frac{\Delta x^2}{3!} + \ldots$$

$$= \frac{u_{i+1} - u_{i-1}}{2\Delta x} + 0(\Delta x^2) \cong \frac{u_{i+1} - u_{i-1}}{2\Delta x} \tag{1.1.10}$$

This is referred to as a central difference approximation to $(du/dx)_i$ and is accurate up to $0(\Delta x^2)$. It is a second-order approximation, or a second approximation to $(du/dx)_i$.

To obtain a finite difference approximation for $(d^2u/dx^2)_i$, one can add Eqs. (1.1.6) and (1.1.7) and solve for $(d^2u/dx^2)_i$. The result is

$$\left(\frac{d^2u}{dx^2}\right)_i = \frac{u_{i+1} - 2u_i + u_{i-1}}{\Delta x^2} - 2\left(\frac{d^4u}{dx^4}\right)_i \frac{\Delta x^2}{4!} \cdots$$

$$= \frac{u_{i+1} - 2u_i + u_{i-1}}{\Delta x^2} + 0(\Delta x^2)$$

$$\cong \frac{u_{i+1} - 2u_i + u_{i-1}}{\Delta x^2} \tag{1.1.11}$$

This is a central difference approximation to $(d^2u/dx^2)_i$ and is a second-order approximation.

It is important to note that, although Eq. (1.1.11) approximates $(d^2u/dx^2)_i$ to $0(\Delta x^2)$, this says nothing about the accuracy of a solution to a difference equation involving this derivative! For example, terms in a difference equation may all be second-order accurate but the difference equation itself may be unstable making accuracy a meaningless word in this context.

For the example problem defined by Eq. (1.1.1), the above arguments lead to the following difference equations:

$$u_{i+1} - 2u_i + u_{i-1} = x_i^{1/2}\,\Delta x^2 \qquad i = 2, 3, \ldots, I-1 \tag{1.1.12}$$

$$u_1 = 0 \tag{1.1.13}$$

$$u_I - u_{I-1} = 0 \tag{1.1.14}$$

Note that differences in the first equation are $0(\Delta^2)$ while the last difference is only $0(\Delta)$. The solution to a set of difference equations is usually only as accurate as the least accurate difference equation of the set and therefore the above set of equations is formally only first-order accurate. The actual accuracy of a set of equations may differ quite drastically from these simple estimates however.

In order to improve the accuracy of the solution as given by Eqs. (1.1.12), (1.1.13), and (1.1.14), a better approximation to $(du/dx)_I$ must be obtained. This can be done as follows. By Taylor series, one can approximate u_{I-1} and u_{I-2} by

$$u_{I-1} = u_I - \left(\frac{du}{dx}\right)_I \Delta x + \left(\frac{d^2u}{dx^2}\right)_I \left(\frac{\Delta x^2}{2}\right) + \dots \tag{1.1.15}$$

$$u_{I-2} = u_I - 2\left(\frac{du}{dx}\right)_I \Delta x + 4\left(\frac{d^2u}{dx^2}\right)_I \left(\frac{\Delta x^2}{2}\right) + \dots \tag{1.1.16}$$

In order to eliminate the $0(\Delta x^2)$ terms, multiply Eq. (1.1.15) by four and subtract Eq. (1.1.16). The result for $(du/dx)_I$ is then

$$\left(\frac{du}{dx}\right)_I = \frac{3u_I - 4u_{I-1} + u_{I-2}}{2\Delta x} + 0(\Delta x^2) \tag{1.1.17}$$

One can then use this expression with $(du/dx)_I = 0$ to replace Eq. (1.1.14). Eqs. (1.1.12), (1.1.13), and (1.1.14) will then be uniformly $0(\Delta x^2)$.

Another approach sometimes used at a boundary is the method of false points. In this approach, fictitious grid points are introduced which extend beyond the original