FINITE ELEMENTS AND APPROXIMATION

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PREFACE

Today the finite element method is a powerful tool for the approximate solution of differential equations governing diverse physical phenomena. Its use in industry and research is extensive, and indeed it could be said that without it (and its handmaiden the computer) many problems would be incapable of solution. Despite this extensive use, comprehension of the principles involved is often lacking in the user who has been trained in a standard undergraduate course (and indeed in many postgraduate courses). It is the object of this book to address such an audience and to form the background text for an undergraduate or early postgraduate course on the subject. For some years now at the authors' institution a large part of this book has formed the basis of a course given to students of civil engineering, and we find that the principles are readily absorbed. When writing the text the authors kept in mind a wider audience of engineers and physicists, and the coverage is therefore suitable for a broad range of students.

It is now about 25 years since the phrase "finite element method" was coined. At the time its inspiration was the field of structural analysis, and analogies with such a discrete process were used for the solution of continuum problems. As the understanding of the basic process grew, its roots in other mathematical approximation methods (such as those due to Rayleigh, Ritz, and Galerkin) became obvious, and the generality opened up made the field an attractive one for mathematicians. Unfortunately, much of their work is couched in a language that others find difficult to follow. Therefore, in this book we attempt a presentation which, though reasonably rigorous, should be readily understood by those with a basic knowledge of calculus.

Many alternative numerical approximation processes existed before the advent of the finite element method. Here boundary solution techniques and finite difference methods have established their own useful existence—and proponents of these have at times crossed swords with those advocating finite element methods in claiming particular superiority. Today some of us see the essential unity of all approximation processes used in the solution of problems defined by differential equations, and in this book we stress this throughout. We endeavor to show that a "generalized finite element method" can be defined embracing all the alternative variants, thus leaving scope for choosing the "optimal approximation" to the user. For this reason the book begins with a chapter on finite difference methods—probably the most obvious (and oldest) of the approximation procedures.

We have endeavored to provide a sufficient number of illustrative examples as well as exercises to make this a suitable teaching text (or a self-study book). Any suggestions from the reader on detailed improvement of these will be welcome.

Finally, we should like to thank Dr. Don Kelly for contributing the major part of Chapter 8 on error estimates and the secretaries of the Civil Engineering Department at Swansea who typed the manuscript.

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CHAPTER ONE

Continuum Boundary Value Problems and the Need for Numerical Discretization. Finite Difference Methods

1.1. INTRODUCTION

While searching for a quantitative description of physical phenomena, the engineer or the physicist establishes generally a system of ordinary or partial differential equations valid in a certain region (or domain) and imposes on this system suitable boundary and initial conditions. At this stage the mathematical model is complete, and for practical applications "merely" a solution for a particular set of numerical data is needed. Here, however, come the major difficulties, as only the very simplest forms of equations, within geometrically trivial boundaries, are capable of being solved exactly with available mathematical methods. Ordinary differential equations with constant coefficients are one of the few examples for which standard solution procedures are available—and even here, with a large number of dependent variables, considerable difficulties are encountered.

To overcome such difficulties and to enlist the aid of the most powerful tool developed in this century—the digital computer—it is necessary to recast the problem in a purely algebraic form, involving only the basic arithmetic operations. To achieve this, various forms of *discretization* of the continuum problem defined by the differential equations can be used. In such a discretization the infinite set of numbers representing the unknown function or functions is replaced by a finite number of unknown parameters, and this process, in general, requires some form of approximation.

Of the various forms of discretization which are possible, one of the simplest is the *finite difference process*. In this chapter we describe some of the essentials of this process to set the stage, but the remainder of this book is concerned with various *trial function* approximations falling under the general classification of *finite element methods*. The reader will find later that even the finite difference process can be included as a subclass of this more general category.

Before proceeding further we shall focus our attention on some particular problems which will serve as a basis for later examples. It is clearly impossible to deal in detail in a book of this length with a wide range of physical problems, each requiring an introduction to its background. It is our hope, however, that the few examples chosen will serve to introduce the general principles of approximation, which the readers can then apply to their own particular special cases.

1.2. SOME EXAMPLES OF CONTINUUM PROBLEMS

Consider the example of Fig. 1.1*a* in which a problem of heat flow in a two-dimensional domain Ω is presented. If the heat flowing in the direction of the x and y axes per unit length and in unit time is denoted by q_x and q_y respectively, the difference D between outflow and inflow for an element of size $dx\,dy$ is given as

$$D = dy\left(q_x + \frac{\partial q_x}{\partial x}dx - q_x\right) + dx\left(q_y + \frac{\partial q_y}{\partial y}dy - q_y\right) \tag{1.1}$$

For conservation of heat, this quantity must be equal to the sum of the heat generated in the element in unit time, say, $Q\,dx\,dy$, where Q may vary with position and time, and the heat released in unit time due to the temperature change, namely, $-\rho c(\partial\phi/\partial t)\,dx\,dy$, where c is the specific heat, ρ is the density and $\phi(x, y, t)$ is the temperature distribution. Clearly, this requirement of equality leads to the differential relationship

$$\frac{\partial q_x}{\partial x} + \frac{\partial q_y}{\partial y} - Q + \rho c\frac{\partial \phi}{\partial t} = 0 \tag{1.2}$$

which has to be satisfied throughout the problem domain Ω.

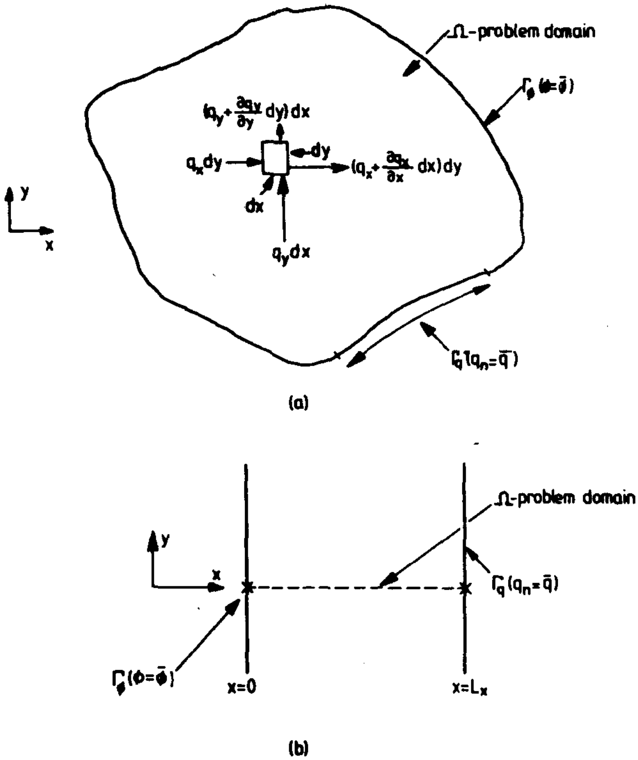

FIGURE 1.1. Examples of continuum problems. (*a*) Two-dimensional heat conduction. (*b*) One-dimensional heat conduction.

Introducing now a physical law governing the heat flow in an isotropic medium,[1] we can write, for the flow component in any direction n,

$$q_n = -k\frac{\partial \phi}{\partial n} \tag{1.3}$$

where k is a property of the medium known as the conductivity. Specifically, in the x and y directions we can then write for an isotropic material

$$\begin{aligned} q_x &= -k\frac{\partial \phi}{\partial x} \\ q_y &= -k\frac{\partial \phi}{\partial y} \end{aligned} \tag{1.4}$$

Relationships (1.2) and (1.4) define a system of differential equations governing the problem at hand, and which now requires solution for the three dependent variables q_x, q_y, and ϕ.

Such a solution needs the specification of *initial conditions* at time, say, $t = t_0$ (e.g., the distribution of temperature may be given everywhere in Ω at this time) and of *boundary conditions* on the surface or boundary Γ of the problem. Typically two different kinds of boundary condition may be involved.

In the first condition, say applicable on a portion Γ_ϕ of the boundary, the values of the temperature are specified as $\bar{\phi}(x, y, t)$, so we have

$$\phi - \bar{\phi} = 0 \qquad \text{on } \Gamma_\phi . \tag{1.5}$$

A boundary condition of this form is frequently referred to as being a Dirichlet boundary condition.

In the second condition, applicable on the remainder Γ_q of the boundary, the values of the heat outflow in the direction n normal to the boundary are prescribed as $\bar{q}(x, y, t)$. Then we can write

$$q_n - \bar{q} = 0 \qquad \text{on } \Gamma_q \tag{1.6a}$$

or, alternatively,

$$-k\frac{\partial \phi}{\partial n} - \bar{q} = 0 \qquad \text{on } \Gamma_q \tag{1.6b}$$

This type of boundary condition is often called a Neumann boundary condition.

The problem now is completely defined by Eq. (1.2), (1.4), (1.5), and (1.6), and numbers representing the distribution of ϕ, q_x, and q_y at all times can, in principle, be obtained by the solution of this set of equations.

This problem may be expressed in an alternative form by using Eq. (1.4) to eliminate the quantities q_x and q_y from Eq. (1.2), and now a higher order differential equation in a single independent variable results. Performing this elimination produces the equation

$$\frac{\partial}{\partial x}\left(k\frac{\partial \phi}{\partial x}\right) + \frac{\partial}{\partial y}\left(k\frac{\partial \phi}{\partial y}\right) + Q - \rho c\frac{\partial \phi}{\partial t} = 0 \tag{1.7}$$

which once again requires the specification of initial and boundary conditions.

In the above we have been concerned with a problem defined in time and space domains, with the former requiring the specification of initial conditions. The independent variables here were x, y, and t. If *steady-state* conditions are assumed (i.e., the problem is invariant with time and so $\partial/\partial t = 0$), the governing equation (1.2) or (1.7) simplifies. In the latter case we have

$$\frac{\partial}{\partial x}\left(k\frac{\partial \phi}{\partial x}\right) + \frac{\partial}{\partial y}\left(k\frac{\partial \phi}{\partial y}\right) + Q = 0 \tag{1.8}$$

which for solution requires only the imposition of boundary conditions of the form (1.5) and (1.6). Such boundary value problems will be the subject of discussion of the major part of this book, but in Chapter 7 we shall return to time-dependent equations and consider possible methods for their solution.

While we have written here the governing equations for a two-dimensional situation, this could have easily been extended to three dimensions to deal with more general problems. On the other hand, in some problems only a one-dimensional variation occurs; in Fig. 1.1*b*, for instance, we consider the heat flow through a slab in which conditions do not vary with y. Then, from Eq. (1.8), we have for steady state an ordinary differential equation

$$\frac{d}{dx}\left(k\frac{d\phi}{dx}\right) + Q = 0 \tag{1.9}$$

and the problem "domain" is now simply the range $0 \leqslant x \leqslant L_x$.

Such an ordinary differential equation can be solved analytically, but we shall use it and similar equations extensively to illustrate the application of discretization procedures. This will enable us to demonstrate the accuracy of approximate methods by comparing their results with the exact solutions.

The problem of heat flow just described is typical of many other physical situations and indeed can be identified with problems such as the following.

1. Irrotational ideal fluid flow. If we put $k = 1$, $Q = 0$, then Eq. (1.8) reduces to a simple Laplacian form;

$$\frac{\partial^2\phi}{\partial x^2} + \frac{\partial^2\phi}{\partial y^2} \equiv \nabla^2\phi = 0 \tag{1.10}$$

   which is the equation governing the distribution of the potential in irrotational ideal fluid flow.
2. Flow of fluid through porous media. Here we take $Q = 0$ and identify k as the medium permeability. The hydraulic head ϕ then satisfies Eq. (1.8).
3. Small deformation of membranes under a lateral load. With $k = 1$ and Q defined to be the ratio of the lateral load intensity to the in-plane tension of the membrane, Eq. (1.8) is the equation governing the transverse membrane deflection ϕ.

Other applications will occur to the reader familiar with different physical and engineering problems, and from time to time we shall introduce in this book different applications of the above differential equation and indeed other systems of differential equations.

Although at such times the full exploration of the origin and derivation of such equations may not always be apparent to all readers, we hope that the procedures of mathematical discretization adopted to produce a solution will be clear in each case.

1.3. FINITE DIFFERENCES IN ONE DIMENSION

Suppose we are faced with a simple one-dimensional boundary value problem, that is, we wish to determine a function $\phi(x)$ which satisfies a given differential equation in the region $0 \leqslant x \leqslant L_x$, together with appropriate boundary conditions at $x = 0$ and $x = L_x$. As we have just seen, a typical example of this type of problem would be that of calculating the temperature distribution $\phi(x)$ through a slab of thickness L_x, of thermal conductivity k, with the faces $x = 0$ and $x = L_x$ maintained at given temperatures $\bar{\phi}_0$ and $\bar{\phi}_{L_x}$, respectively, and with heat generation at a rate $Q(x)$ per unit length in the slab. The governing differential equation for this problem is given by Eq. (1.9), which reduces to the equation

$$k\frac{d^2\phi}{dx^2} = -Q(x) \tag{1.11}$$

if we make the assumption that the material thermal conductivity is constant. The associated boundary conditions are of the type given in Eq. (1.5) and can be written as

$$\phi(0) = \bar{\phi}_0, \qquad \phi(L_x) = \bar{\phi}_{L_x} \tag{1.12}$$

To solve this problem by the finite difference method we begin by *differencing* the independent variable x, that is, we construct a set (or *grid* or *mesh*) of $L + 1$ discrete, equally spaced grid points x_l ($l = 0, 1, 2, \ldots, L$) on the range $0 \leqslant x \leqslant L_x$ (see Fig. 1.2) with $x_0 = 0$, $x_L = L_x$, and $x_{l+1} - x_l = \Delta x$.

The next step is to replace those terms in the differential equation that involve differentiation by terms involving algebraic operations only. This process, of necessity, involves an approximation and can be accomplished by making use of the finite difference approximations to function derivatives. The manner in which such approximations can be made are now discussed.

1.3.1. The Finite Difference Approximation of Derivatives

Using Taylor's theorem with remainder we can write, exactly,

$$\phi(x_{l+1}) = \phi(x_l + \Delta x) = \phi(x_l) + \Delta x\left.\frac{d\phi}{dx}\right|_{x=x_l} + \frac{\Delta x^2}{2}\left.\frac{d^2\phi}{dx^2}\right|_{x=x_l+\theta_1\Delta x} \tag{1.13}$$

where θ_1 is some number in the range $0 \leqslant \theta_1 \leqslant 1$. Using the subscript l to

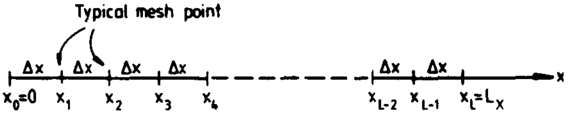

FIGURE 1.2. Construction of a finite difference mesh over the interval $0 \leqslant x \leqslant L_x$.

denote an evaluation at $x = x_l$, this can be written

$$\phi_{l+1} = \phi_l + \frac{\Delta x}{2} \frac{d\phi}{dx}\bigg|_l + \frac{\Delta x^2}{2} \frac{d^2\phi}{dx^2}\bigg|_{l+\theta_1} \tag{1.14}$$

and therefore

$$\frac{d\phi}{dx}\bigg|_l = \frac{\phi_{l+1} - \phi_l}{\Delta x} - \frac{\Delta x}{2} \frac{d^2\phi}{dx^2}\bigg|_{l+\theta_1} \tag{1.15}$$

This leads to the so-called *forward difference* approximation of the first derivative of a function in which

$$\frac{d\phi}{dx}\bigg|_l \approx \frac{\phi_{l+1} - \phi_l}{\Delta x} \tag{1.16}$$

The error E in this approximation can be seen to be given by

$$E = -\frac{\Delta x}{2} \frac{d^2\phi}{dx^2}\bigg|_{l+\theta_1} \tag{1.17}$$

and as E is equal to a constant multiplied by Δx, we say that this error is $O(\Delta x)$. This is known as the *order* of the error.

The exact magnitude of the error cannot be obtained from this expression, as the actual value of θ_1 is not given by Taylor's theorem, but it follows that

$$|E| \leqslant \frac{\Delta x}{2} \max_{[x_l, x_{l+1}]} \left|\frac{d^2\phi}{dx^2}\right| \tag{1.18}$$

Figure 1.3 shows a graphical interpretation of the approximation that we have derived mathematically. The first derivative of $\phi(x)$ at $x = x_l$ is the slope of the tangent to the curve $y = \phi(x)$ at this point, that is, the slope of the line AB. The forward difference approximation is the slope of the line AC, and it can be seen that the slope of this line approaches that of the line AB as the mesh spacing Δx gets smaller.

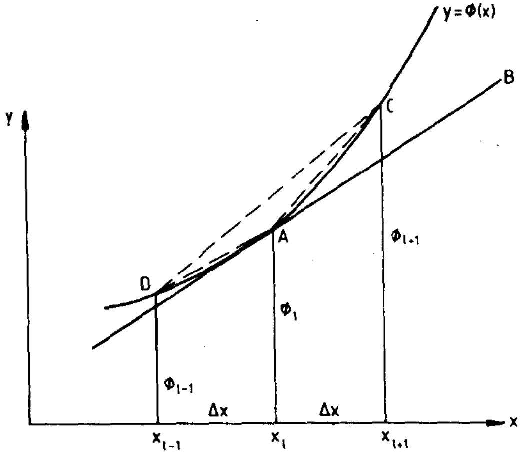

FIGURE 1.3. A graphical interpretation of some finite difference approximations to $d\phi/dx|_l$. Forward difference—slope of AC; backward difference—slope of DA; central difference—slope of DC.

In a similar manner we can use Taylor's theorem to obtain

$$\phi_{l-1} = \phi_l - \Delta x \left.\frac{d\phi}{dx}\right|_l + \frac{\Delta x^2}{2} \left.\frac{d^2\phi}{dx^2}\right|_{l-\theta_2} \tag{1.19}$$

where $0 \leqslant \theta_2 \leqslant 1$. Rewriting this expression in the form

$$\left.\frac{d\phi}{dx}\right|_l = \frac{\phi_l - \phi_{l-1}}{\Delta x} + \frac{\Delta x}{2} \left.\frac{d^2\phi}{dx^2}\right|_{l-\theta_2} \tag{1.20}$$

we can produce the *backward difference* approximation

$$\left.\frac{d\phi}{dx}\right|_l \simeq \frac{\phi_l - \phi_{l-1}}{\Delta x} \tag{1.21}$$

The error E in this approximation is again $O(\Delta x)$, and now

$$|E| \leqslant \frac{\Delta x}{2} \max_{[x_{l-1}, x_l]} \left|\frac{d^2\phi}{dx^2}\right| \tag{1.22}$$

The graphical representation of the backward difference approximation can be seen in Figure 1.3; the slope of the line AB is now approximated by the slope of the line AD.

In both the forward and the backward difference approximations the error is of the same order, that is, $O(\Delta x)$. However, if we replace the expansions of