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COMPUTATIONAL METHODS FOR PDE IN MECHANICS

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COMPUTATIONAL METHODS FOR PDE IN MECHANICS

To my wife Silvana
and my daughters Lucia and Erica

Preface

Several physical phenomena are governed by partial differential equations. Obviously, this is not a mere chance. Indeed, scientists and technicians, following the scientific method introduced by Galilei, know very well that every natural event can be analyzed by means of a related mathematical model. This is very often based on partial differential equations. A celebrated and historical example is given by the Maxwell equations, which admirably describe the electro-magnetic field. Other emblematic, not less important, models are: Fourier (heat) equation, D'Alembert (wave) equation, Laplace/Poisson (potential) equation, Euler/Stokes (fluid) equations.

Mathematical modeling has been successively adopted by researchers working in several other fields and so, at present, partial differential equations can help to explain phenomena occurring in Biology, Medicine, Economy, Sociology, and so on.

During the last two hundred years, applied mathematician involved in the above topic have never ended. The first pioneers concentrated their efforts on the exact solutions. Next, the attention was focused on the qualitative analysis in order to obtain information on the solutions even when these could not be explicitly found. In the last sixty years, also the quantitative analysis has been strongly developed in parallel with the great growth of computers power. At present, numerical methods provide a powerful approach for solving partial differential equations and their knowledge becomes more and more a necessary cultural luggage of applied researchers and technicians.

This book is an elementary introduction to computational methods, based on the finite differences, for parabolic, hyperbolic and elliptic partial differential equations. The numerical discussion of each type of equation is always preceded by the introduction of models in Mechanics, which are carefully derived. In particular, the role of the initial and boundary conditions is pointed out with reference to physical situations. The numerical analysis is concerned with the most used finite-difference methods for each type of equation. Several examples are solved and exercises proposed to give the Reader the opportunity to practice. Since there is no numerical method without approximations, the accuracy of the schemes is also analyzed. Special attention is devoted to the propagation of rounding errors, which inevitable arise during the computational process. This leads to discuss the basic concepts of stability, consistency and convergence, which are illustrated by inductive procedures and then formalized.

Dealing with applied numerical methods sooner or later requires that own programs have to be developed. Therefore, some examples are provided by using the C++ language. The classic C language was evolved after 1970 by B. W. Kernigham and D. M. Ritchie. C++, developed by B. Stroustrup in 1980s, is an extension of C. It provides the capabilities of object-oriented programming. It is considered the most powerful and flexible language. The Visual C++ [1] compiler is quickly introduced and Windows [2] programs are built step by step. These programs can be easily fitted to other situations, with small changes. The codes of the programs developed in this book are also supplied with the enclosed CD-Rom.

Chapter 1 deals with the most used finite-difference approximations of derivatives. In particular, the forward, central and backward approximations are derived. Chapter 2 presents the classical model of heat conduction in solids, based on Fourier law. Also, phase-change problems are illustrated. Chapter 3 introduces the classical explicit method for the one-dimensional heat equation. The concepts of stability, consistency and convergence are applied. Developing programs in C++, related to the heat equation, is the topic of Chapters 4 and 5. Chapter 6 describes numerical methods for parabolic equations. Some nonlinear case is also considered and a melting problem is discussed. Furthermore, the classical explicit method is generalized to the heat equation in two and three space dimensions. A program related to this case is developed in Chapter 7. Chapter 8 is devoted to wave motions. At first, the wave equation is derived from the model of one-dimensional continuum. Next, we introduce the equations governing the motions of general continuous systems. As special cases the elastic and fluid media are examined in order to point out wave phenomena. Finally, a free-boundary value problem is presented. Explicit and implicit finite-

[1] Visual C++ is a registered trademark of Microsoft Corporation
[2] Windows is a registered trademark of Microsoft Corporation

difference methods for the wave equation are illustrated in Chapter 9. An example of third-order equation is provided. Chapter 10 deals with finite-difference methods for linear and nonlinear hyperbolic systems. Elliptic equations are considered in Chapter 11. The motions of fluids through porous media are examined. In Appendix A the classification of partial differential equations is given for second-order equations and general systems of first-order equations. Elements of Linear Algebra are briefly provided in Appendix B.

The author is grateful to Professor N. Bellomo for encouraging him to write this book and the pertinent suggestions, for reading the manuscript and making various useful criticisms.

Especial thanks are due to World Scientific Publishing Co.

B. D'Acunto

University of Naples "Federico II", 2004.

About the CD

The CD contains the complete source code of the three projects from the book. Each project has a separate subdirectory on the CD: Heat1, Heat2, Heat3. To compile any project, just copy it on the hard disk in a suitable subdirectory, for example, C: Projects.

The executable files are also supplied, so that the programs can be used without compiling. To run a program, double-click the related file. Furthermore, the User will find the files where the data related to the examples were saved.

Contents

Chapter 1

Finite differences

The scientific community agrees that finite-difference schemes were first used by Euler (1707-1783) to find approximate solutions of differential equations. The technique is known as *Euler method.* However, only after 1945 systematic research activity on the above topic has been strongly developed, when high-speed computers began to be available.

At present, finite-difference methods provide a powerful approach to solve differential equations and are widely used in any field of applied sciences. Equations with variable coefficients and even nonlinear problem can be treated by these techniques. Generally, the error of an approximating solution can be made arbitrary small. Rounding errors, which inevitably arise during the computational process, can be controlled by a preliminary analysis of the numerical stability of finite-difference schemes. Furthermore, numerical solutions can give suggestions to more general questions.

This chapter introduces to the most used finite-difference approximations of derivatives. In particular, the well-known forward, central and backward approximations are presented. The analysis systematically starts from Taylor's series expansion so that the truncation error can be immediately pointed out. Firstly, the approximation of first-order derivatives is dealt with, and, subsequently, the analysis is developed for higher-order derivatives. Exercises are proposed to give the Reader the opportunity to practice. Finally, we present some finite-difference operators, which are frequently found in literature. Their use can help to shorten long formulas in some cases.

1.1 Function discretization

Let us consider a function $u(x,t)$ depending on two variables $x \in [0,L]$ and $t \in [0,T]$. A discretization of function u is obtained by considering only the values $u_{i,j}$ on a finite number of points (x_i, t_j)

$$u_{i,j} = u(x_i, t_j) = u(i\Delta x, j\Delta t), \; i = 0, ..., m, \; j = 0, ..., n, \tag{1.1.1}$$

where $\Delta x = L/m$, $\Delta t = T/n$, fig. 1.1.1. Usually, instead of $u_{i,j}$, the notation u_i^j is also used.

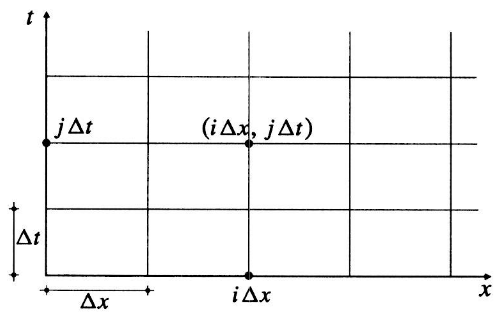

Fig. 1.1.1 Space-time grid

The formula for a function of one variable is immediately derived from (1.1.1). In addition, generalizing it in obvious way yields the case regarding a function of three or more variables.

A basic role to estimate the error involved in *finite-difference approximations* of function derivatives is played by the well-known Taylor's series expansion

$$f(x+\Delta x) = f(x) + \sum_{h=1}^{n-1} f^{(h)}(x)\frac{(\Delta x)^h}{h!} + f^{(n)}(x+\theta\Delta x)\frac{(\Delta x)^n}{n!}, \tag{1.1.2}$$

where $0 < \theta < 1$ and $f^{(h)}$ denotes the hth derivative of f. Noting that the last term is of order $(\Delta x)^n$, (1.1.2) can also be written as

$$f(x+\Delta x) = f(x) + \sum_{h=1}^{n-1} f^{(h)}(x)\frac{(\Delta x)^h}{h!} + O((\Delta x)^n), \tag{1.1.3}$$

where the symbol O (big o) has been used, defined as follows

$$g(y) = O(y^n), \; y \in \Omega \quad \Leftrightarrow \quad |g(y)| \leq cy^n, \quad \forall y \in \Omega, \tag{1.1.4}$$

where c is a positive constant.

1.2 Finite-difference approximation of derivatives

Let us define the *forward approximation* for the partial derivative u_t. Applying Taylor's series expansion (1.1.3) to $u(x_i, t_j + \Delta t)$ gives

$$u(x_i, t_j + \Delta t) = u(x_i, t_j) + u_t(x_i, t_j)\Delta t + O((\Delta t)^2) \tag{1.2.1}$$

which, by using notation (1.1.1), is written as

$$u_{i,j+1} = u_{i,j} + (u_t)_{i,j}\Delta t + O((\Delta t)^2), \tag{1.2.2}$$

that is,

$$(u_t)_{i,j} = \frac{u_{i,j+1} - u_{i,j}}{\Delta t} + O(\Delta t). \tag{1.2.3}$$

Hence, it follows the approximation formula for the partial derivative of u with respect to t, called *forward approximation*,

$$(u_t)_{i,j} \approx \frac{u_{i,j+1} - u_{i,j}}{\Delta t}. \tag{1.2.4}$$

Formula (1.2.4) evidently implies a leading error of order Δt. Similarly, from

$$(u_x)_{i,j} = \frac{u_{i+1,j} - u_{i,j}}{\Delta x} + O(\Delta x) \tag{1.2.5}$$

it follows the forward approximation for u_x

$$(u_x)_{i,j} \approx \frac{u_{i+1,j} - u_{i,j}}{\Delta x}, \tag{1.2.6}$$

with a leading error of order Δx.

The *backward approximation* is inferred in analogous way. Applying Taylor's expansion (1.1.3) to $u(x_i, t_j - \Delta t)$ and $u(x_i - \Delta x, t_j)$ implies, respectively, the following

$$(u_t)_{i,j} \approx \frac{u_{i,j} - u_{i,j-1}}{\Delta t}, \tag{1.2.7}$$

$$(u_x)_{i,j} \approx \frac{u_{i,j} - u_{i-1,j}}{\Delta x}, \tag{1.2.8}$$

which give the *backward approximations* for the first partial derivatives, with the same leading error of the last case.

Let us define the *central approximation*. Applying Taylor's expansion (1.1.3) with $n = 4$ yields

$$u_{i,j+1} = u_{i,j} + (u_t)_{i,j}\Delta t + (u_{tt})_{i,j}\frac{(\Delta t)^2}{2!} + (u_{ttt})_{i,j}\frac{(\Delta t)^3}{3!} + O((\Delta t)^4), \quad (1.2.9)$$

$$u_{i,j-1} = u_{i,j} - (u_t)_{i,j}\Delta t + (u_{tt})_{i,j}\frac{(\Delta t)^2}{2!} - (u_{ttt})_{i,j}\frac{(\Delta t)^3}{3!} + O((\Delta t)^4). \quad (1.2.10)$$

Subtracting the second expression from the first gives

$$u_{i,j+1} - u_{i,j-1} = 2(u_t)_{i,j}\Delta t + O((\Delta t)^3), \quad (1.2.11)$$

that is,

$$(u_t)_{i,j} = \frac{u_{i,j+1} - u_{i,j-1}}{2\Delta t} + O((\Delta t)^2). \quad (1.2.12)$$

Hence, we obtain the *central approximation* for u_t

$$(u_t)_{i,j} \approx \frac{u_{i,j+1} - u_{i,j-1}}{2\Delta t}, \quad (1.2.13)$$

with a leading error of order $(\Delta t)^2$. Similarly, it follows

$$(u_x)_{i,j} = \frac{u_{i+1,j} - u_{i-1,j}}{2\Delta x} + O((\Delta x)^2). \quad (1.2.14)$$

Hence,

$$(u_x)_{i,j} \approx \frac{u_{i+1,j} - u_{i-1,j}}{2\Delta x}, \quad (1.2.15)$$

which gives the central approximation for u_x with the same error.

The preceding finite-difference approximations consider the values of a function on two points of the xt grid and are the most used. However, formulas involving three or more grid points can also be deduced with a smaller error, in general. Firstly, let us discuss the *three-point forward approximation* for u_t. Using again Taylor's expansion (1.1.3) gives

$$u_{i,j+1} - u_{i,j} = (u_t)_{i,j}\Delta t + (u_{tt})_{i,j}(\Delta t)^2/2 + O((\Delta t)^3), \quad (1.2.16)$$

$$u_{i,j+2} - u_{i,j} = (u_t)_{i,j}2\Delta t + (u_{tt})_{i,j}2(\Delta t)^2 + O((\Delta t)^3), \quad (1.2.17)$$