Numerical Methods
in Scientific Computing

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Preface

This is a book about numerically solving partial differential equations occurring in technical and physical contexts and we (the authors) have set ourselves a more ambitious target than to just talk about the numerics. Our aim is to show the place of numerical solutions in the general modeling process and this must inevitably lead to considerations about modeling itself. Partial differential equations usually are a consequence of applying first principles to a technical or physical problem at hand. That means, that most of the time the physics also have to be taken into account especially for validation of the numerical solution obtained.

This book in other words is especially aimed at engineers and scientists who have 'real world' problems and it will concern itself less with pesky mathematical detail. For the interested reader though, we have included sections on mathematical theory to provide the necessary mathematical background. Since this treatment had to be on the superficial side we have provided further reference to the literature where necessary.

Delft, June 2005

Jos van Kan
Guus Segal
Fred Vermolen

Note to the first edition improvements

In this improved first edition exercises and theory are more separately presented. Furthermore, some parts, such as the parts on boundary fitted coordinates, on coordinate transformation, the treatment of essential boundary conditions for FEM and the solution of non-linear systems of equations, have been rewritten to make them easier to understand.
Newmark-type solvers for the wave equation have been added.

Delft, April 2008

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Note to the second edition improvements

In this improved second edition the treatment of boundary conditions for all types of discretization methods has been extended. Periodical boundary conditions have been included. Furthermore,the description of the FEM has been simplified.

Delft, August 2014

Guus Segal
Fred Vermolen

Contents

Chapter 1

Review of some basic mathematical concepts

1.1 Preliminaries

In this chapter we take a bird's eye view of the contents of the book. Furthermore we establish a physical interpretation of certain mathematical notions, operators and theorems. As a first application we formulate a general conservation law, since conservation laws are the back bone of physical modeling. Finally we treat some mathematical theorems, that will be used in the remainder of this book.

1.2 Global contents of the book

We first take a look at second order partial differential equations and their relation with various physical problems. Then we look at numerical methods for those equations. First we look at finite difference methods, of respectable age but still very much in use. Subsequently we take on finite volume methods, a typical engineers option, constructed for conservation laws. Finally we turn to finite element methods (FEM) which have gained tremendous popularity over the last decades. Before we can move to FEM, however, we have to delve a bit into minimization problems to provide a proper background. We shall show, that FEM may be considered as a special case of Ritz's method, a particular way of obtaining an approximate solution to a minimization problem. We shall establish a relation between minimization problems and partial differential equations. But not all PDEs can be formulated as a minimization problem and we shall consider a generalization that will enable us to apply the FEM also to those problems.

These methods generally leave us with a large set of linear or non-linear equations and we consider ways of how to solve them. In particular we shall pay some attention to efficient methods that are relatively young, like preconditioned Krylov space methods and multi-grid methods. The treatment can be only cursory but further references will be provided.

We also pay some attention to special methods for specific problems like heat and wave equations. Finally we consider transport equations. They do not fall within the previous context, being only first order, yet they are very important and deserve a chapter of their own. The last chapter will be dedicated to miscellaneous problems that fall outside the classification so far.

Chapter 2

A crash course in PDE's

Objectives

In the previous chapter we looked at PDE's from the *modeling* point of view, but now we shall look at them from a *mathematical* angle. Apparently you need partial derivatives and at least *two* independent variables to speak of a PDE (with fewer variables you would have an ordinary differential equation), so the simplest case to consider is a PDE with exactly two independent variables. A second aspect is the *order* of the PDE, that is the order of the highest derivative occurring in it. First order PDE's are a class of their own: the *transport* equations. We shall consider them in Chapter 11. In this chapter we shall take a look at second order PDE's and show that (for two independent variables) they can be classified into three types. We shall provide boundary and initial conditions that are needed to guarantee a unique solution and we will consider a few properties of the solutions to these PDE's. We conclude the chapter with a few examples of second and fourth order equations that occur in various fields of physics and technology.

2.1 Classification

Consider a second order PDE in two independent variables *with constant coefficients.*

$$a_{11}\frac{\partial^2 u}{\partial x^2} + 2a_{12}\frac{\partial^2 u}{\partial x \partial y} + a_{22}\frac{\partial^2 u}{\partial y^2} + b_1\frac{\partial u}{\partial x} + b_2\frac{\partial u}{\partial y} + cu + d = 0. \tag{2.1.1}$$

By *rotating* the coordinate system we can make the term with the mixed second derivative vanish. This is the basis of the classification. To carry out this rotation, we keep in mind that

$$(\frac{\partial}{\partial x}, \frac{\partial}{\partial y})A\begin{pmatrix}\frac{\partial u}{\partial x}\\ \frac{\partial u}{\partial y}\end{pmatrix} = a_{11}\frac{\partial^2 u}{\partial x^2} + 2a_{12}\frac{\partial^2 u}{\partial x \partial y} + a_{22}\frac{\partial^2 u}{\partial y^2}, \tag{2.1.2}$$

where $A = \begin{pmatrix} a_{11} & a_{12} \\ a_{12} & a_{22} \end{pmatrix}$. Since A is symmetric, we can factorize A into $A = Q\Lambda Q^T$, where $\Lambda = \text{diag}\,(\alpha_{11}, \alpha_{22})$, in which α_{11} and α_{22} are eigenvalues of A. The columns of Q are the normalized (with length one) eigenvectors of A. Note that $Q^T = Q^{-1}$

Chapter 3

Finite difference methods

Objectives

In this chapter we shall look at the form of discretization that has been used since the days of Euler (1707-1783): finite difference methods. To grasp the essence of the method we shall first look at some one dimensional examples. After that we consider two-dimensional problems on a *rectangle* because that is a straightforward generalization of the one dimensional case. We take a look at the discretization of the three classical types of boundary conditions. After that we consider more general domains and the specific problems at the boundary. Finally we shall turn our attention to the solvability of the resulting discrete systems and the convergence towards the exact solution.

3.1 The cable equation

As an introduction we consider the displacement y of a cable under a vertical load. (See Figure 3.1)

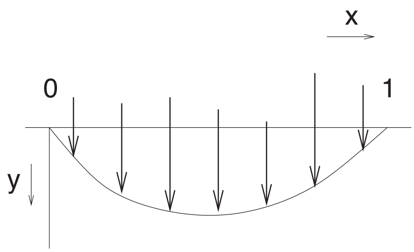

Figure 3.1: Loaded cable.

This problem is described mathematically by the second order ordinary differential equation:

$$-\frac{d^2y}{dx^2} = f, \tag{3.1.1}$$

and since the cable has been fixed at both ends we have a Dirichlet boundary condition at each boundary point:

$$y(0) = 0, \quad y(1) = 0. \tag{3.1.2}$$

Note that here also *one* boundary condition is necessary for the whole boundary, which just consists of two points.