Numerical Methods in Scientific Computing



Jos van Kan (1944) graduated in 1968 from Delft University of Technology, Delft, Netherlands, in Numerical Analysis and has been assistant professor at the Department of Mathematics of that institute ever since. He wrote several articles on Numerical Fuid Mechanics (pressure correction methods) and has written a multigrid pressure solver for the Delft software package to solve the Navier Stokes equations. He has been teaching classes in Numerical Analysis since 1971 and wrote several books on the subject.



Guus Segal (1948) graduated in 1971 from Delft University of Technology, Delft, Netherlands, in Numerical Analysis and has been part time assistant professor at the Department of Mathematics of that institute ever since. He is also working in the consultancy and numerical software company SEPRA in Den Haag, The Netherlands. He wrote a number of articles on Finite Element Methods and several articles on curvilinear Finite Volume Methods and Numerical Fluid Mechanics. He has written a book on Finite Element Methods and Navier-Stokes equations. He is the main developer of the finite element package SEPRAN. He has been teaching classes in Numerical Analysis since 1973.



Fred Vermolen (1969) graduated in 1993 from Delft University of Technology, Delft, Netherlands. He wrote his PhD-thesis supervised by the promotores prof Pieter Wesseling (Numerical Analysis) and prof Sybrand van der Zwaag (Materials Science). He wrote several articles on Stefan problems and transport in porous media. His present interest is in mathematical issues in medicine. He has been teaching courses in Numerical Analysis since 2002.

Numerical Methods in Scientific Computing

J. van Kan, A. Segal, F. Vermolen

Department of Applied Mathematics Delft University of Technology

© VSSD First edition 2005, improved 2008

Published by VSSD Leeghwaterstraat 42, 2628 CA Delft, The Netherlands tel. +31 15 27 82124, telefax +31 15 27 87585, e-mail: hlf@vssd.nl internet: http://www.vssd.nl/hlf URL about this book: http://www.vssd.nl/hlf/a002.htm

All rights reserved. No part of this publication may be reproduced, stored in a retrieval system, or transmitted, in any form or by any means, electronic, mechanical, photocopying, recording, or otherwise, without the prior written permission of the publisher.

Printed version ISBN-13 978-90-71301-50-6 Electronic version ISBN-13 978-90-6562-179-5

NUR 919

Key words: numerical mathematics

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

Jos van Kan Guus Segal Fred Vermolen

Contents

Pr	Preface v					
1 Modelling						
	1.1	Preliminaries	1			
	1.2	Global contents	1			
	1.3	Building blocks for mathematical modelling	1			
		1.3.1 Gradient of a scalar	2			
		1.3.2 Directional derivative	4			
		1.3.3 Divergence of a vector field	4			
		1.3.4 Gauss' divergence theorem	5			
		1.3.5 Conservation laws	7			
	1.4	Minimization	8			
		1.4.1 Elastic string	8			
	1.5	Summary of Chapter 1	9			
2	A cr	ash course in PDE's	10			
-		ctives	10			
	2.1	Classification	10			
		2.1.1 Three or more independent variables	12			
	2.2	Boundary and initial conditions	12			
		2.2.1 Boundary conditions	13			
		2.2.2 Initial conditions	14			
	2.3	Existence and uniqueness of a solution	14			
		2.3.1 The Laplacian operator	15			
		2.3.2 The maximum principle	15			
		2.3.3 Existence	17			
	2.4	Examples	17			
		2.4.1 Flows driven by a potential	18			
		2.4.2 Convection-Diffusion	18			
		2.4.3 Navier-Stokes equations	19			
		2.4.4 Plane stress	20			
		2.4.5 Biharmonic equation	22			
	2.5	Summary of Chapter 2	23			

3		Finite difference methods 24						
	Obje	ctives	4					
	3.1	The cable equation	4					
		3.1.1 Discretization	4					
		3.1.2 Global error	6					
	3.2	Singularly perturbed problems	8					
		3.2.1 Analytical solution	8					
		3.2.2 Numerical approximation	8					
	3.3	The Laplacian equation on a rectangle	2					
		3.3.1 Matrix vector form	3					
	3.4	Boundary conditions extended	5					
		3.4.1 Natural boundary conditions	5					
		3.4.2 Dirichlet boundary conditions on non rectangular regions 33	5					
	3.5	Global error estimate						
		3.5.1 A discrete maximum principle						
		3.5.2 Super solutions						
	3.6	Boundary fitted coordinates						
	3.7	Summary of Chapter 3						
	5.7		5					
4	Fini	te volume methods 44	4					
	Obje	ctives	4					
	4.1	Heat transfer with varying coefficient	4					
		4.1.1 The boundaries	6					
		4.1.2 Conservation	6					
		4.1.3 Error in the temperatures	7					
	4.2	Laplacian equation in 2 dimensions	8					
		4.2.1 Boundary cells on straight boundaries	9					
		4.2.2 Error considerations in the interior	0					
		4.2.3 Error considerations at the boundary	1					
	4.3	Laplacian in general coordinates	1					
		4.3.1 Discrete transformation from Cartesian to General coordinates 5	1					
		4.3.2 An example of finite volume integration in polar co-ordinates 53	3					
		4.3.3 Boundary conditions	4					
		4.3.4 Error analysis						
	4.4	Finite volumes on two component fields						
		4.4.1 Staggered grids						
		4.4.2 Boundary conditions						
	4.5	Project: Stokes equations for incompressible flow						
	4.6	Summary of Chapter 4						
	1.0		5					
5	Min	mization problems in physics 64	4					
	Obje	ctives	4					
	5.1	Introduction	4					
		5.1.1 Minimal potential energy	4					
		5.1.2 Derivation of the differential equation	5					

	5.2	0 1		
	5.3	A sim	ble two-dimensional case	69
	5.4	Examp	bles of minimization problems	71
		5.4.1	Minimal surface problem	71
		5.4.2	Minimal potential energy	72
		5.4.3	Small displacement theory of elasticity (Plane stress)	73
		5.4.4	Loaded and clamped plate	74
	5.5		dimensional problem	75
	5.6	Theore	tical remarks	75
		5.6.1	Smoothness requirements	75
		5.6.2	Boundary conditions	76
		5.6.3	Weak formulation	76
	5.7	Exerci	ses	77
		PDE to minimization problem	78	
		5.8.1	Introduction	78
		5.8.2	Linear problems with homogeneous boundary conditions	79
		5.8.3	Linear problems with non-homogeneous boundary conditions	81
		5.8.4	Exercises	83
	5.9	Mathe	matical theory of minimization	84
	5.10		ary of Chapter 5	87
6			cal solution of minimization problems	88
	Ohie	ctives		88
	6.1	Ritz's	method	88
		Ritz's 6.1.1	method	88 88
		Ritz's 6.1.1 6.1.2	method	88 88 89
		Ritz's 6.1.1 6.1.2 6.1.3	method	88 88 89 91
	6.1	Ritz's 6.1.1 6.1.2 6.1.3 6.1.4	method	88 88 89 91 93
		Ritz's 6.1.1 6.1.2 6.1.3 6.1.4 The fir	method	88 88 89 91 93 95
	6.1	Ritz's 6.1.1 6.1.2 6.1.3 6.1.4 The fir 6.2.1	method	88 88 89 91 93 95 95
	6.1	Ritz's 6.1.1 6.1.2 6.1.3 6.1.4 The fir 6.2.1 6.2.2	method	88 88 89 91 93 95 95 95
	6.1	Ritz's 6.1.1 6.1.2 6.1.3 6.1.4 The fir 6.2.1 6.2.2 6.2.3	method	 88 89 91 93 95 95 95 98
	6.1	Ritz's 6.1.1 6.1.2 6.1.3 6.1.4 The fin 6.2.1 6.2.2 6.2.3 6.2.4	method	88 89 91 93 95 95 95 95 98 99
	6.1	Ritz's 6.1.1 6.1.2 6.1.3 6.1.4 The fir 6.2.1 6.2.2 6.2.3 6.2.4 6.2.5	method	88 89 91 93 95 95 95 98 99 101
	6.1	Ritz's 6.1.1 6.1.2 6.1.3 6.1.4 The fin 6.2.1 6.2.2 6.2.3 6.2.4 6.2.5 6.2.6	method	88 89 91 93 95 95 95 98 99 101 102
	6.1	Ritz's 6.1.1 6.1.2 6.1.3 6.1.4 The fir 6.2.1 6.2.2 6.2.3 6.2.4 6.2.5	method	88 89 91 93 95 95 95 98 99 101 102 104
	6.1	Ritz's 6.1.1 6.1.2 6.1.3 6.1.4 The fir 6.2.1 6.2.2 6.2.3 6.2.4 6.2.5 6.2.6 6.2.7 6.2.8	method	88 89 91 93 95 95 95 98 99 101 102 104 106
	6.1	Ritz's 6.1.1 6.1.2 6.1.3 6.1.4 The fir 6.2.1 6.2.2 6.2.3 6.2.4 6.2.5 6.2.6 6.2.7 6.2.8	methodIntroductionA simple one-dimensional example	88 89 91 93 95 95 95 98 99 101 102 104 106
	6.1	Ritz's 6.1.1 6.1.2 6.1.3 6.1.4 The fir 6.2.1 6.2.2 6.2.3 6.2.4 6.2.5 6.2.6 6.2.7 6.2.8	methodIntroductionA simple one-dimensional example	88 89 91 93 95 95 95 98 99 101 102 104 106
	6.1	Ritz's 6.1.1 6.1.2 6.1.3 6.1.4 The fir 6.2.1 6.2.2 6.2.3 6.2.4 6.2.5 6.2.6 6.2.7 6.2.8 The fir	methodIntroductionA simple one-dimensional example	88 88 91 93 95 95 95 98 99 101 102 104 106 106
	6.1	Ritz's 6.1.1 6.1.2 6.1.3 6.1.4 The fir 6.2.1 6.2.2 6.2.3 6.2.4 6.2.5 6.2.6 6.2.7 6.2.8 The fir 6.3.1	method	88 89 91 93 95 95 95 98 99 101 102 104 106 106 106 108 111
	6.1	Ritz's 6.1.1 6.1.2 6.1.3 6.1.4 The fir 6.2.1 6.2.2 6.2.3 6.2.4 6.2.5 6.2.6 6.2.7 6.2.8 The fir 6.3.1 6.3.2	method	88 89 91 93 95 95 95 98 99 101 102 104 106 106 106 108 111
	6.1	Ritz's 6.1.1 6.1.2 6.1.3 6.1.4 The fir 6.2.1 6.2.2 6.2.3 6.2.4 6.2.5 6.2.6 6.2.7 6.2.8 The fir 6.3.1 6.3.2 6.3.3 6.3.4	method	88 88 91 93 95 95 95 98 99 101 102 104 106 106 106 108 111 112
	6.16.26.3	Ritz's 6.1.1 6.1.2 6.1.3 6.1.4 The fir 6.2.1 6.2.2 6.2.3 6.2.4 6.2.5 6.2.6 6.2.7 6.2.8 The fir 6.3.1 6.3.2 6.3.3 6.3.4	method	88 88 91 93 95 95 95 98 99 101 102 104 106 106 106 108 111 112 114

		6.4.3 Approximation errors	. 117
	6.5	Summary of Chapter 6	. 117
7	The	weak formulation and Galerkin's method	119
	7.1	The weak formulation for a symmetrical problem	
	/11	7.1.1 Introduction	
		7.1.2 Natural boundary conditions	
		7.1.3 Non-homogeneous essential boundary conditions	
	7.2	The weak formulation for a non-symmetric problem	
	7.3	Galerkin's method	
		7.3.1 Introduction	
		7.3.2 Galerkin's method applied to the convection-diffusion equation	
		7.3.3 The convection-diffusion equation in \mathbb{R}^1 by finite elements	
		7.3.4 The convection-diffusion equation in \mathbb{R}^2 by finite elements	
	7.4	Petrov-Galerkin	
		7.4.1 Introduction	
		7.4.2 Upwinding in \mathbb{R}^1 by Petrov-Galerkin	
		7.4.3 SUPG: stream line upwinding in \mathbb{R}^2 by Petrov-Galerkin	
	7.5	An example of a system of coupled PDEs	
	7.6	Mathematical theory	
	7.7	Summary of Chapter 7	
8	Exte	ension of the FEM	136
U			
	8.1	(Straight) quadratic triangles	
	8.2	Quadrilaterals	
	8.3	Curved quadratic triangles	
	8.4	Application to the Stokes equations	
	8.5	Circle symmetry	
	86	Theoretical remarks	
	8.6 8.7	Theoretical remarks	. 148
	8.6 8.7	Fourth order problems	. 148 . 150
		Fourth order problems	. 148 . 150 . 150
		Fourth order problems	. 148 . 150 . 150 . 152
0	8.7 8.8	Fourth order problems	. 148 . 150 . 150 . 152 . 153
9	8.7 8.8 Solu	Fourth order problems	 . 148 . 150 . 150 . 152 . 153 154
9	8.7 8.8 Solu Obje	Fourth order problems	 . 148 . 150 . 150 . 152 . 153 154 . 154
9	8.7 8.8 Solu	Fourth order problems	. 148 . 150 . 150 . 152 . 153 154 . 154
9	8.7 8.8 Solu Obje	Fourth order problems	. 148 . 150 . 150 . 152 . 153 154 . 154 . 154 . 154
9	8.7 8.8 Solu Obje	Fourth order problems	 . 148 . 150 . 150 . 152 . 153 154 . 154 . 154 . 154 . 155
9	8.7 8.8 Solu Obje	Fourth order problems	 . 148 . 150 . 150 . 152 . 153 154 . 154 . 154 . 155 . 157
9	8.7 8.8 Solu Obje	Fourth order problems	 . 148 . 150 . 150 . 152 . 153 154 . 154 . 154 . 155 . 157 . 159
9	8.7 8.8 Solu Obje	Fourth order problems	. 148 . 150 . 150 . 152 . 153 154 . 154 . 154 . 154 . 155 . 157 . 159 . 160

	9.2	Generi	c iterative process		164
	9.3	Defect	correction		164
		9.3.1	Algorithm		164
		9.3.2	Convergence of defect correction		164
		9.3.3	Error estimate for defect correction		165
		9.3.4	Estimate of the spectral radius		166
		9.3.5	M-matrices		166
	9.4	Classic	cal preconditioners		167
		9.4.1	Jacobi		
		9.4.2	Gauss-Seidel		168
		9.4.3	Successive Overrelaxation SOR		169
		9.4.4	Block variations		171
		9.4.5	Operation count		171
	9.5	Krylov	y space methods		172
		9.5.1	Introduction		172
		9.5.2	The Krylov space		174
		9.5.3	Conjugate gradients		174
		9.5.4	CG algorithm		175
		9.5.5	Preconditioning		177
		9.5.6	Convergence		178
		9.5.7	Krylov space methods for non symmetric matrices		180
		9.5.8	Preconditioners		181
	9.6	The m	ultigrid algorithm		184
		9.6.1	A one-dimensional example		184
		9.6.2	Smooth and rough part of the spectrum		
		9.6.3	Two grid algorithm		187
		9.6.4	From two grid to multigrid		
		9.6.5	Convergence of the two grid algorithm		190
		9.6.6	Restriction and prolongation in two dimensions		
		9.6.7	Concluding remarks about MG		193
	9.7	Non-li	near equations		
		9.7.1	Picard iteration		193
		9.7.2	Newton's method in more dimensions		195
		9.7.3	Starting values		197
	9.8	Summa	ary of Chapter 9		198
10	The	haat- ai	r diffusion equation		199
10					199
			lamental inequality		
			d of lines		
	10.2		One dimensional examples		
			Two-dimensional example		
	10.3		tency of the spatial discretization		
			ntegration		
	10.5	Stabili	ty of the numerical integration	•••	208
				- •	

C	ont	ents
· ·	Uni	CIUS

		10.5.1 Gershgorin's circle theorem	
		10.5.2 Stability analysis of Von Neumann	
		The accuracy of the time integration	
		Conclusions for the method of lines	
	10.8	Special difference methods for the heat equation	215
		10.8.1 The principle of the ADI method	215
		10.8.2 Formal description of the ADI method	217
	10.9	Summary of Chapter 10	218
11		wave equation	220
	•	ctives	
	11.1	A fundamental equality	220
	11.2	The method of lines	
		11.2.1 The error in the solution of the system	222
		Numerical time integration	
	11.4	Stability of the numerical integration	225
		Total dissipation and dispersion	
	11.6	Direct time integration of the second order system	228
	11.7	The CFL criterion	231
	11.8	Summary of Chapter 11	233
12		transport equation	234
	Obje	ctives	234
	12.1	Introduction	234
	12.2	Characteristics	235
	12.3	Some classical numerical procedures	237
		12.3.1 Central discretization and upwind discretization	238
	12.4	Mathematical theory for the transport equation	246
		12.4.1 Burgers equation	246
		12.4.2 The Buckley-Leverett equation	249
	12.5	Summary of Chapter 12	258
	12.6	Appendix: requirements on flux-limiters	258
13	Mov	ing boundary problems	261
		ctives	
	13.1	The formulation of a classical Stefan problem: ice and water	261
	13.2	An exact (self-similar) solution for an unbounded region	263
	13.3	Numerical methods	264
		13.3.1 Moving grid methods	265
		13.3.2 A fixed domain method: the level set method	269
		13.3.3 Other applications of Stefan problems	276
	13.4	Summary of Chapter 13	
Bił	oliogr	aphy	278

Chapter 1

Modelling

1.1 Preliminaries

In this first chapter we shall take a bird's eye view of the contents of the book and try to establish what topics are of interest to which reader. Furthermore we shall establish a physical interpretation of certain mathematical notions, operators and theorems, because this really permeates the whole modelling process. As a first application we shall formulate a general conservation law, because conservation laws are the back bone of physical modelling.

1.2 Global contents

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, tailor made for conservation laws. And finally we turn to finite element methods (FEM) which have gained tremendous popularity over the last three 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 multigrid 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.

1.3 Building blocks for mathematical modelling

Several mathematical concepts used in modelling are directly derived from a physical context. We shall consider a few of those and see how they can be used to formulate a fundamental mathematical model: conservation.

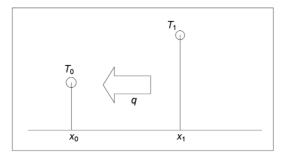


Figure 1.1 1-dimensional heat flow.

1.3.1 Gradient of a scalar

The mathematical definition of gradient is uninspiring. Given a scalar function u of two variables, differentiable with respect to both variables the gradient is defined as

$$\operatorname{grad} u = \begin{pmatrix} \frac{\partial u}{\partial x} \\ \frac{\partial u}{\partial y} \end{pmatrix}.$$
 (1.3.1)

Instead of the notation grad u also ∇u (pronounce: nabla u) is used. To get to the core of what a gradient really is, think of temperature. If you have a temperature difference between two points you get a flow of heat between those points that only will stop when the temperature difference has been annihilated. If the difference is bigger, the flow will be larger. If the points are closer together the flow will be larger. The simplest one dimensional model to reflect this is the following linear model. Let q be the generated flow, directly proportional to the temperature difference ΔT and inversely proportional to the distance Δx . This leads to:

$$q = -\lambda \ \frac{\Delta T}{\Delta x},\tag{1.3.2}$$

where λ is a material constant, the *heat conduction* coefficient. The minus sign reflects the facts that

- 1. heat flows from high to low temperatures
- 2. physicists hate negative constants

In a continuous temperature field T(x) we may take limits and obtain a flow that is derived from (driven by) the temperature:

$$q = -\lambda \, \frac{dT}{dx}.\tag{1.3.3}$$

How is this in more than one dimension? Suppose we have a two-dimensional temperature field T(x,y) which we can represent nicely by considering the contour lines which for temperature are called *isotherms*, lines that connect points of equal temperature.

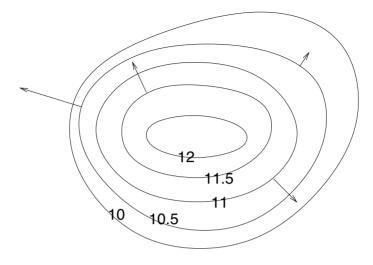


Figure 1.2 Isotherms.

Since there cannot be heat flow between points of equal temperature, the heat flow must be orthogonal to the contour lines at every point. Two vectors **v** and **w** are orthogonal if their inner product (**v**, **w**) vanishes. In other words: let x(s), y(s) be a parameterization of a contour line and let $\begin{pmatrix} q_1 \\ q_2 \end{pmatrix}$ be the components of the heat flow field. We then have:

$$q_1 \frac{dx}{ds} + q_2 \frac{dy}{ds} = 0. (1.3.4)$$

at every point x(s), y(s) of the isotherm, for all isotherms. Let us substitute the equation of an isotherm into the temperature field: T(x(s), y(s)). Doing this makes T a function of s only, which is constant because we are on an isotherm. In other words along an isotherm:

$$\frac{dT}{ds} = \frac{\partial T}{\partial x}\frac{dx}{ds} + \frac{\partial T}{\partial y}\frac{dy}{ds} = 0.$$
(1.3.5)

If we compare Equation (1.3.4) with (1.3.5) we see that these can only be satisfied if

$$\mathbf{q} = -\lambda \,\operatorname{grad} T. \tag{1.3.6}$$

For three dimensions you can tell basically the same story that also ends in Equation 1.3.6. This is known as *Fourier's law* and it is at the core of the theory of heat conduction.

Exercise 1.3.1 (*Darcy's Law*). In ground water flow the velocities are very small, a few centimeters per day. This makes ground water flow basically a hydrostatic problem, in which the flow is driven by differences in hydrostatic pressure. This hydrostatic pressure depends linearly on the height of the ground water level h. So how does the flow \mathbf{q} depend on h?

Exercise 1.3.2 (Fick's Law) In diffusion the flow of matter \mathbf{q} is driven by differences in concentration c. Express \mathbf{q} in c.

Scalar fields like T, h and c that drive a gradient flow field \mathbf{q} are called *potentials*. Not all flow fields are generated by the gradient of a potential. But those that are, are called *solenoidal* or *irrotational*.

Exercise 1.3.3 Let C be a closed contour in the x-y-plane and \mathbf{q} a solenoidal vector field. Show that $\int_{C} \mathbf{q} \cdot d\mathbf{s} = 0$.

1.3.2 Directional derivative

In the previous paragraph we saw, how the temperature *T* changes along a curve x(s), y(s). The actual value of $\frac{dT}{ds}$ depends on the parameterization. A natural parameterization is the *arc length* of the curve. Note, that in that case $(\frac{dx}{ds})^2 + (\frac{dy}{ds})^2 = 1$. This forms the basis of the following definition:

Definition 1.3.1 Let \mathbf{n} be a unit vector, then the directional derivative of T in the direction of \mathbf{n} is given by

$$\frac{\partial T}{\partial n} = \frac{\partial T}{\partial x} n_1 + \frac{\partial T}{\partial y} n_2 = (\operatorname{grad} T, \mathbf{n}) = (\mathbf{n} \cdot \nabla) T.$$

Exercise 1.3.4 Compute the directional derivative of $z = x^2 + y^3$ in (1,1) in the direction (1,-1). (Answer: $-\frac{1}{2}\sqrt{2}$).

Exercise 1.3.5 For what value of **n** is the directional derivative precisely $\frac{\partial T}{\partial x}$?

1.3.3 Divergence of a vector field

The mathematical definition of divergence is equally uninspiring. Given a continuously differentiable vector field $\begin{pmatrix} v_1 \\ v_2 \end{pmatrix}$ the divergence of **v** is defined by:

div
$$\mathbf{v} = \frac{\partial v_1}{\partial x} + \frac{\partial v_2}{\partial y}.$$
 (1.3.7)

For \mathbb{R}^3 you have the obvious generalization and there is also a nabla notation: div $\mathbf{v} = \nabla \cdot \mathbf{v}$. You will appreciate the correspondence of a genuine inner product of two vectors and the inner product of the "nabla vector" and a vector field. Take care, however. In a genuine inner product you can change the order of the vectors, in the divergence you cannot.

What is the physical meaning of divergence? You could think of a vector field as a river: at any place in the river the water has a certain velocity with direction and magnitude. Now consider a fixed rectangular volume in the river (see Figure 1.3).

Water is flowing in through the left and bottom wall and flowing out through the right and top wall. How much is flowing *in* through the left wall? If you think about it, you will notice that the *y*-component of the velocity gives no contribution to the inflow, because that is parallel to the left wall. So the inflow through the left wall is equal to $v_{1L}L_y$, the outflow through the right wall $v_{1R}L_y$. By the same reasoning the inflow through the bottom equals $v_{2R}L_x$, the outflow through the top equals $v_{2T}L_x$. What's left behind? If the

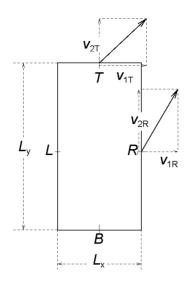


Figure 1.3 Square volume in river.

net outflow is larger than the net inflow we are losing matter in the volume, if on the other hand the net inflow is larger we're gaining. The net outflow is given by

$$\Phi_{net} = v_{1R}L_y - v_{1L}L_y + v_{2T}L_x - v_{2B}L_x, = \left(\frac{v_{1R} - v_{1L}}{L_x} + \frac{v_{2T} - v_{2B}}{L_y}\right)L_xL_y,$$
(1.3.8)
 $\approx \operatorname{div} \mathbf{v}\Delta V.$

So you may consider a divergence as an outflow density.

Exercise 1.3.6 *Explain that for an* incompressible *flow field* \mathbf{u} *we must have* div $\mathbf{u} = 0.\Box$

Exercise 1.3.7 Derive in the same way as above that divergence is an outflow density in \mathbb{R}^3 .

1.3.4 Gauss' divergence theorem

What we have informally derived in the previous section is stated by Gauss' divergence theorem in a precise way. In words: the outflow density integrated over an arbitrary volume gives the total outflow out of this volume. But this is mathematics, so we have to be more precise.

Theorem 1.3.1 Gauss' divergence theorem.

Let Ω be a bounded domain in \mathbb{R}^2 (\mathbb{R}^3) with piecewise smooth boundary Γ . Let **n** be the outward normal and **v** a continuously differentiable vector field. Then

$$\int_{\Omega} \operatorname{div} \mathbf{v} \, d\Omega = \int_{\Gamma} \mathbf{v} \cdot \mathbf{n} \, d\Gamma. \tag{1.3.9}$$

Remark

- 1. The expression $\mathbf{v} \cdot \mathbf{n}$ is the normal component of the velocity with respect to the boundary. If this is positive you have outflow, otherwise inflow.
- 2. Any good book on multivariate analysis will have a proper proof of Gauss' theorem. (See for instance [2] or [33]). A good insight will be obtained however, by subdividing the region Ω in small rectangles and using (1.3.8). Note in particular, that the common side (plane in \mathbb{R}^3) of two neighboring volumes cancel: what flows out of one flows into the other.

The Divergence theorem has many important implications and these implications are used frequently in various numerical methods, such as the finite element method. First, one can use the component-wise product rule for differentiation to arrive at the following theorem

Theorem 1.3.2 For a continuously differentiable scalar field c and vector field u, we have

$$div (c\mathbf{u}) = grad \ c \cdot \mathbf{u} + c \ div \ \mathbf{u}. \tag{1.3.10}$$

As a result of this, one can prove the following theorem

Theorem 1.3.3 *Green's Theorem For a sufficiently smooth c*, **u**, *we have*

$$\int_{\Omega} c \operatorname{div} \mathbf{u} \, d\Omega = -\int_{\Omega} (\operatorname{grad} c) \cdot \mathbf{u} d\Omega + \oint_{\Gamma} c \mathbf{u} \cdot \mathbf{n} \, d\Gamma.$$
(1.3.11)

Exercise 1.3.8 Prove Theorem 1.3.2.

Exercise 1.3.9 Prove Theorem 1.3.3.

By the use of Theorem 1.3.3, the following assertion can be demonstrated:

Theorem 1.3.4 *Partial integration in 2 D For sufficiently smooth scalar functions* ϕ *and* ψ *, we have;*

$$\int_{\Omega} \phi \frac{\partial \psi}{\partial x} \, d\Omega = -\int_{\Omega} \frac{\partial \phi}{\partial x} \psi \, d\Omega + \oint_{\Gamma} \phi \psi n_1 d\Gamma, \qquad (1.3.12)$$

and

$$\int_{\Omega} \phi \frac{\partial \psi}{\partial y} \, d\Omega = -\int_{\Omega} \frac{\partial \phi}{\partial y} \psi \, d\Omega + \oint_{\Gamma} \phi \psi n_2 d\Gamma.$$
(1.3.13)

Exercise 1.3.10 Prove Theorem 1.3.4.

Hint: choose an appropriate vector field \mathbf{u} *in the previous exercise.* \Box

1.3.5 Conservation laws

Let us consider some flow field **u** in a volume V with boundary Γ . If the net inflow into this volume is positive *something* in this volume must increase (whatever it is). That is the basic form of a conservation law:

$$\frac{\partial}{\partial t} \int_{V} S \, dV = -\int_{\Gamma} \mathbf{u} \cdot \mathbf{n} \, d\Gamma + \int_{V} f(t, \mathbf{x}) \, dV. \tag{1.3.14}$$

The term $f(t, \mathbf{x})$ is a production *density*, it tells how much *S* is produced any time, any place within *V*. The boundary integral describes the net inflow into *V* (mark the minus sign). The flow field **u** is also called the *flux vector* of the model. *S* just like *f* has the dimension of a *density*. Since Equation (1.3.14) has to hold for every conceivable volume in the flow field we may formulate a *point wise* conservation law as follows. First we apply Gauss' Theorem 1.3.9 to Equation ((1.3.14)) to obtain

$$\frac{\partial}{\partial t} \int_{V} S dV = -\int_{V} \operatorname{div} \mathbf{u} \, dV + \int_{V} f(t, \mathbf{x}) \, dV.$$
(1.3.15)

Subsequently we invoke the mean-value theorem of integral calculus for each integral separately, assuming all integrands are continuous:

$$\frac{\partial S}{\partial t}(\mathbf{x}_1) = -\operatorname{div} \mathbf{u}(\mathbf{x}_2) + f(t, \mathbf{x}_3).$$
(1.3.16)

Observe that we have divided out a factor $\int_V dV$ and that \mathbf{x}_1 , \mathbf{x}_2 and \mathbf{x}_3 all lie within *V*. Finally we let *V* contract to a single point \mathbf{x} to obtain a point wise conservation law in the form of a PDE:

$$\frac{\partial S}{\partial t} = -\operatorname{div} \mathbf{u} + f(t, \mathbf{x}). \tag{1.3.17}$$

This is all rather abstract, so let us look at an example.

1.3.5.1 Example: Heat flow

In heat flow, conservation law (1.3.17) takes the form

$$\frac{\partial h}{\partial t} = -\operatorname{div} \mathbf{q} + f(t, \mathbf{x}), \qquad (1.3.18)$$

in which h is the heat density, \mathbf{q} the heat flux vector and f the production density. Remember, that all quantities in such a point wise conservation law are densities. The heat density h stored in a material can be related to the materials (absolute) temperature T:

$$h = \rho cT, \tag{1.3.19}$$

in which ρ is the density and *c* the heat capacity of the material. These material properties have to be measured. As we already saw in Section 1.3.1 the heat flow **q** is driven by the temperature gradient: $\mathbf{q} = -\lambda \nabla T$. This enables us to formulate everything in terms of temperature. Substituting this all we get:

$$\frac{\partial \rho cT}{\partial t} = \operatorname{div} \lambda \,\operatorname{grad} T + f(t, \mathbf{x}). \tag{1.3.20}$$

If ρ , *c* are constant throughout the material and if there is no internal heat production this transforms into the celebrated heat conduction equation:

$$\frac{\partial T}{\partial t} = \operatorname{div}(k \operatorname{grad} T), \qquad (1.3.21)$$

with $k = \lambda / (\rho c)$.

1.4 Minimization

Another way of deriving models is by looking at the potential energy. This is most often used in mechanical problems, but can also be used in different contexts. An equilibrium state can be found by minimizing that potential energy. We also meet minimization problems in optics (optical length) and economics (cost).

1.4.1 Elastic string

As an example consider an elastic string fixed in (0,0) and (0,1), see Figure 1.4.

Without load, the string is undeformed: u(x) = 0. When we apply a load *f* the string deforms. What is the potential energy of the deformed string? First of all, there is an elastic energy proportional to the increase in length: $\Delta P_e = k\Delta L$. Over a small interval Δx this increase amounts to

$$\Delta L = \sqrt{\Delta x^2 + \Delta u^2 - \Delta x}.$$
 (1.4.1)

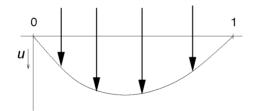


Figure 1.4 Deformed elastic string.

When the inclination $\Delta u/\Delta x$ is small (this is true in a realistic problem), this is approximately equal to

$$\Delta L = \Delta x \left(1 + \frac{1}{2} \left(\frac{\Delta u}{\Delta x}\right)^2\right) - \Delta x, \qquad (1.4.2)$$

$$=\frac{1}{2}\left(\frac{\Delta u}{\Delta x}\right)^2 \Delta x. \tag{1.4.3}$$

The work done by the load f per fragment Δx equals $\Delta W = uf\Delta x$, assuming we take the positive u-axis pointing down. The potential energy per fragment Δx then is given by $\Delta P_e - \Delta W$ and the potential energy over the whole string is obtained by integrating over the whole interval (0,1):

$$P = P_e - W = \int_0^1 \frac{1}{2}k \left(\frac{du}{dx}\right)^2 - uf \, dx.$$
(1.4.4)

So any (sufficiently smooth) function u satisfying u(0) = 0 and u(1) = 0 yields a potential energy. The solution to the mechanical problem is that function u for which the potential energy P is minimal. In Chapter 5 we shall see how to deal with this.

Exercise 1.4.1 Show by Taylor's theorem that $\sqrt{1+x} = 1 + \frac{1}{2}x + O(x^2)$.

1.5 Summary of Chapter 1

In this chapter we have seen the importance of conservation in the development of models and the role the mathematical operators *divergence* and *gradient* play in that development. We have met the famous divergence theorem of Gauss as an expression of global conservation.

We have looked at various applications deriving from conservation: heat transfer, diffusion and ground water flow. We concluded the chapter with an example of minimization as an instrument to derive a physical model.

Chapter 2

A crash course in PDE's

Objectives

In the previous chapter we looked at PDE's from the *modelling* point of view, but now we shall look at them from a *mathematical* angle. Apparently you need at least *two* independent variables to speak of a PDE (with less you would have an ordinary differential equation), so the simplest case to consider are PDE's 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 needed to guarantee a unique solution and consider a few properties of 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.

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

$$\left(\frac{\partial}{\partial x}, \frac{\partial}{\partial y}\right) A \left(\frac{\partial u}{\partial x}\right) = a_{11} \frac{\partial^2 u}{\partial x^2} + 2a_{12} \frac{\partial^2 u}{\partial x \partial y} + a_{22} \frac{\partial^2 u}{\partial y^2}, \qquad (2.1.2)$$

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 $Q^T = Q^{-1}$ due to symmetry of *A*. Hence, one obtains from equation (2.1.2)

$$a_{11}\frac{\partial^{2}u}{\partial x^{2}} + 2a_{12}\frac{\partial^{2}u}{\partial x\partial y} + a_{22}\frac{\partial^{2}u}{\partial y^{2}} = \left(\frac{\partial}{\partial x}, \frac{\partial}{\partial y}\right)Q\Lambda Q^{T}\left(\frac{\partial u}{\partial x}\right) = \left(\frac{\partial}{\partial \xi}, \frac{\partial}{\partial \eta}\right)\Lambda\left(\frac{\partial u}{\partial \xi}\right) = \alpha_{11}\frac{\partial^{2}u}{\partial \xi^{2}} + \alpha_{22}\frac{\partial^{2}u}{\partial \eta^{2}}.$$
(2.1.3)

The resulting equation will look like:

$$\alpha_{11}\frac{\partial^2 u}{\partial\xi^2} + \alpha_{22}\frac{\partial^2 u}{\partial\eta^2} + \beta_1\frac{\partial u}{\partial\xi} + \beta_2\frac{\partial u}{\partial\eta} + cu + d = 0.$$
(2.1.4)

Exercise 2.1.1 Show that $a_{12}^2 - a_{11}a_{22} < 0$, $a_{12}^2 - a_{11}a_{22} = 0$ and $a_{12}^2 - a_{11}a_{22} > 0$, respectively correspond to $\alpha_{11}\alpha_{22} > 0$, $\alpha_{11}\alpha_{22} = 0$ and $\alpha_{11}\alpha_{22} < 0$ (these cases correspond to the situations in which the eigenvalues of A have the same sign, one of the eigenvalues of A is zero and opposite signs of the eigenvalues of A respectively).

There are three possibilities:

1. $\alpha_{11}\alpha_{22} > 0$. (I.e. both coefficients have the same sign) The equation is called *elliptic*. An example of this is *Poisson's equation*

$$\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} = f.$$
(2.1.5)

2. $\alpha_{11}\alpha_{22} < 0$. (I.e. both coefficients have opposite sign) The equation is called *hyperbolic*. An example of this is the wave equation

$$\frac{\partial^2 u}{\partial x^2} - \frac{\partial^2 u}{\partial y^2} = 0.$$
(2.1.6)

3. $\alpha_{11}\alpha_{22} = 0$. (I.e. either coefficient vanishes). The equation is called *parabolic*. An example is the heat equation in one space dimension:

$$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2}.$$
(2.1.7)

Exercise 2.1.2 Let $D = a_{11}a_{22} - a_{12}^2$. Show that the condition for hyperbolic, parabolic or elliptic in the original coefficients a_{ij} is given by D < 0, D = 0 and D > 0 respectively. Use the result of Exercise 2.1.1.

For the classification only the second order part of the PDE is important. The three different types have very different physical and mathematical properties. To begin with, elliptic equations are time-independent and often describe an equilibrium. Parabolic and hyperbolic equations are time-dependent: they describe the evolution in time or *transient behavior* of a process.

This classification strictly spoken only holds for equations with constant coefficients. For equations with varying coefficients this classification holds only *locally*. If the coefficients depend on the solution itself the type of equation may depend on the solution itself.

2.1.1 Three or more independent variables

The general second order part of a *quasi-linear* PDE in N > 2 independent variables is given by:

$$\sum_{i=1}^{N} \sum_{j=1}^{N} a_{ij} \frac{\partial^2 u}{\partial x_i \partial x_j}.$$
(2.1.8)

 $a_{ij} = a_{ji}$ and in a way similar to that in the previous section one may remove the mixed derivatives. This leads to:

$$\sum_{i=1}^{N} \alpha_{ii} \frac{\partial^2 u}{\partial \xi_i^2}.$$
(2.1.9)

Only three cases are of interest in a physical context:

1. All α_{ii} have the same sign. In this case all independent variables ξ_i are space variables. The equation is called *elliptic*. Example: 3D Laplacian

$$\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} + \frac{\partial^2 u}{\partial z^2} = 0.$$
 (2.1.10)

2. Exactly one α_{ii} , say α_{11} has different sign from the rest. In this case ξ_1 is a time variable, all other ξ_i are space variables. The equation is called *hyperbolic*. Example: 3D Wave equation

$$\frac{\partial^2 u}{\partial t^2} = \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} + \frac{\partial^2 u}{\partial z^2}.$$
 (2.1.11)

3. Exactly one α_{ii} vanishes, say α_{11} . Then ξ_1 is a time variable and the equation is called *parabolic*. Example: 3D Heat equation

$$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} + \frac{\partial^2 u}{\partial z^2}.$$
(2.1.12)

Exercise 2.1.3 If A is a symmetric $n \times n$ matrix there exists a real unitary matrix C such that $C^T A C = \Lambda$. Λ is a diagonal matrix containing the eigenvalues of A on the diagonal. Show that the substitution $\xi = C^T \mathbf{x}$ eliminates the mixed derivatives in the differential operator div A grad u.

2.2 Boundary and initial conditions

To ensure a unique solution to our PDE we need to prescribe appropriate boundary conditions and in time dependent problems we need initial conditions too. We will just consider here second order PDE's because the considerations for first order PDE's are very different and will be considered in Chapter 11.

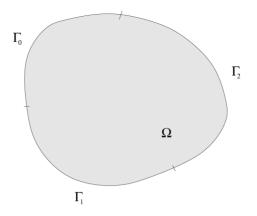


Figure 2.1 The bounded region Ω .

2.2.1 Boundary conditions

Consider the bounded region in \mathbb{R}^2 , Ω with boundary Γ in Figure 2.1. Let Γ consist of three *disjoint* pieces Γ_0 , Γ_1 and Γ_2 . For an elliptic equation of the form

$$\operatorname{div} k \operatorname{grad} u = f, \tag{2.2.1}$$

with $k > 0 \ \forall \mathbf{x} \in \overline{\Omega}$, the following boundary conditions guarantee a unique solution:

1.

$$u = g_0(\mathbf{x}), \quad \mathbf{x} \in \Gamma_0, \tag{2.2.2}$$

the Dirichlet boundary condition.

2.

$$k\frac{\partial u}{\partial n} = g_1(\mathbf{x}), \quad \mathbf{x} \in \Gamma_1, \tag{2.2.3}$$

the Neumann boundary condition.

3.

$$k\frac{\partial u}{\partial n} + \sigma u = g_2(\mathbf{x}), \quad \sigma \ge 0, \ \mathbf{x} \in \Gamma_2,$$
 (2.2.4)

the Robbins, radiation, kinetic or mixed boundary condition.

These boundary conditions do not have to occur together, each (but not all) of Γ_0 , Γ_1 or Γ_2 could be empty. Because the pieces are disjoint exactly *one* boundary condition occurs on each point of the boundary. There is a small problem if $\Gamma = \Gamma_1$ in other words if there is a Neumann boundary condition on all of the boundary. Physically this may be understood, by noting that the *inflow* at each point of the boundary is prescribed. And since we have an equilibrium the net inflow over the whole region must be annihilated inside or the net outflow must be produced inside. This result is stated in mathematical form in the following theorem.

Theorem 2.2.1 If a Neumann boundary condition is given on all of Γ , then the solution *u* of Equation (2.2.1) is determined up to an additive constant only. Moreover the following compatibility condition must be satisfied:

$$\int_{\Gamma} g_1 d\Gamma = \int_{\Omega} f d\Omega \qquad (2.2.5)$$

Exercise 2.2.1 *Prove Theorem 2.2.1. Use Gauss' divergence theorem on the PDE.*

Remarks

- 1. Only the highest order part of the PDE determines what type of boundary conditions are needed, so the same set is needed if first and zeroth order terms are added to Equation (2.2.1).
- 2. On each part of the boundary *precisely one* boundary condition applies. (For second order PDE's)
- 3. Boundary conditions involving the flux vector (Neumann, Robbins) are also called *natural boundary conditions*. (For second order PDE's) This term will be explained in Chapter 5.
- 4. The boundary conditions needed in parabolic and hyperbolic equations are determined by the spatial part of the equation.
- 5. If the coefficients of the terms of the highest order are *very small* compared to the coefficients of the lower order terms it is to be expected that the nature of the solution is mostly determined by those lower order terms. Such problems are called *singularly perturbed*. An example is the convection dominated convection-diffusion equation.

2.2.2 Initial conditions

Initial conditions only play a role in time dependent problems, and we can be very short. If the equation is first order in time, *u* has to be given on all of Ω at $t = t_0$. If the equation is second order in time in addition $\frac{\partial u}{\partial t}$ has to be given on all of Ω at $t = t_0$.

Exercise 2.2.2 Consider the transversal vibrations of membrane that is fixed to an iron ring. These vibrations are described by the wave equation. What is the type of boundary condition? What initial conditions are needed?

2.3 Existence and uniqueness of a solution

Physicists and technicians usually consider the mathematical chore of proving existence and uniqueness of a solution a waste of time. 'I know the process behaves in precisely one way', they will claim and of course they are right in that. What they do not know is if their mathematical model describes their process with any accuracy and existence and uniqueness of a solution is an acid test for that. In ODE's a practical way to go about this is try and find one. In PDE's this is not much of an option, since solutions in closed form are seldom available.

Proving existence and uniqueness is usually a very difficult assignment, but to get some of the flavor we shall look at a relatively simple example: Poisson's Equation (2.1.5). We shall prove that a solution to this equation with Dirichlet boundary conditions on all of Γ is unique.

2.3.1 The Laplacian operator

The Laplacian operator div grad is such a fundamental operator that it has a special symbol in the literature: Δ . So the following notations are equivalent:

div grad
$$u \equiv \Delta u \equiv \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2}.$$
 (2.3.1)

In a technical context div grad is mostly used, in mathematical contexts the other two.

2.3.2 The maximum principle

Solutions to Laplace's and Poisson's equation share a number of properties that have to do with extreme values in the interior of Ω . To start off, we note, that if a smooth function of two variables $u(\mathbf{x})$ has an isolated maximum in some point \mathbf{x}_0 (i.e. $u(\mathbf{x}_0) > u(\mathbf{x})$ in a neighborhood of \mathbf{x}_0) then the *Hessian* matrix, that is the matrix of second derivatives (2.3.3), must be negative definite. To prove this, we consider the 2-D Taylor expansion of u around \mathbf{x}_0 :

$$u(\mathbf{x}) = u(\mathbf{x}_0) + \nabla u(\mathbf{x}_0) \cdot (\mathbf{x} - \mathbf{x}_0) + (\mathbf{x} - \mathbf{x}_0, H(\mathbf{x}_0)(\mathbf{x} - \mathbf{x}_0)) + O(||\mathbf{x} - \mathbf{x}_0||^3), \quad (2.3.2)$$

in which H is the Hessian matrix

$$H = \begin{pmatrix} \frac{\partial^2 u}{\partial x^2} & \frac{\partial^2 u}{\partial x \partial y} \\ \frac{\partial^2 u}{\partial y \partial x} & \frac{\partial^2 u}{\partial y^2} \end{pmatrix}.$$
 (2.3.3)

Because *u* has a maximum in \mathbf{x}_0 , $\nabla u(x_0) = \mathbf{0}$. For **x** close enough to \mathbf{x}_0 , say $||\mathbf{x} - \mathbf{x}_0|| < \delta$ the third order term is negligible compared to the rest. Since $u(\mathbf{x}_0) > u(\mathbf{x})$ for all **x** with $||\mathbf{x} - \mathbf{x}_0|| < \delta$, we necessarily have $(\mathbf{x} - \mathbf{x}_0, H(\mathbf{x}_0)(\mathbf{x} - \mathbf{x}_0)) < 0$ for those **x**. Hence $H(\mathbf{x}_0)$ is negative definite.

Exercise 2.3.1 *Prove that* $H(\mathbf{x}_0)$ *is positive definite if u has a minimum in* \mathbf{x}_0 .

Exercise 2.3.2 Show that if H is positive definite both diagonal elements must be positive. *Hint: Make special choices for* \mathbf{u} *in* $(\mathbf{u}, H\mathbf{u})$.

Definition 2.3.1 A function satisfying Laplace's equation $\Delta u = 0$ is called harmonic.

The result of Exercise 2.3.2 shows that if a function of two variables f has an isolated minimum both f_{xx} and f_{yy} must be positive. This suggests the following theorem on harmonic functions :

Theorem 2.3.1 If $u(\mathbf{x})$ is harmonic in a bounded region Ω , then u cannot have an extreme value in an interior point of Ω .

To prove this theorem the observations on the Hessian are insufficient, we need something more. Harmonic functions have a number of interesting properties, one of which is described by

Lemma 2.3.2 Let u be harmonic in Ω . Let \mathbf{x}_0 be a point of Ω and let C be a circular disk with midpoint \mathbf{x}_0 , radius r and boundary ∂C fully contained in Ω . Then $r^{-1} \int_{\partial C} u \, ds$ does not depend on r and is equal to $2\pi u(\mathbf{x}_0)$.

Proof By Gauss' divergence theorem we have

$$\int_{C} \operatorname{div}\operatorname{grad} u \, d\Omega = \int_{\partial C} \frac{\partial u}{\partial r} \, ds, \qquad (2.3.4)$$

where *r* represents the distance between any point in *C* and \mathbf{x}_0 . Since *u* is harmonic the integral on the left side vanishes, so

$$\int_{\partial C} \frac{\partial u}{\partial r} ds = 0.$$
(2.3.5)

Now putting $ds = rd\varphi$ we get $r \int_0^{2\pi} \frac{\partial u}{\partial r} d\varphi = 0$ and hence $\int_0^{2\pi} \frac{\partial u}{\partial r} d\varphi = 0$. Note that the integrand must be evaluated at

$$\mathbf{x} = \mathbf{x}_0 + r \left(\begin{array}{c} \cos \varphi \\ \sin \varphi \end{array}\right).$$

Interchanging the order of integration and differentiation we get

$$\frac{\partial}{\partial r} \int_{0}^{2\pi} u(\mathbf{x}) d\varphi = 0,$$

giving us

$$\int_{0}^{2\pi} u(\mathbf{x}) d\varphi = \text{ constant.}$$

By taking r = 0 we obtain the value of this constant: $2\pi u(\mathbf{x}_0)$.

If a harmonic function has an extreme within Ω , hence not on the boundary, then the function is constant. This is formulated in the following theorem:

Theorem 2.3.3 If a harmonic function u takes on a maximum M at an interior point \mathbf{x}_0 of Ω , then

1. u = M at the circumference of any circle with midpoint \mathbf{x}_0 fully contained in Ω ;

2. u = M on every disk with midpoint \mathbf{x}_0 that is fully contained in Ω ;

3. u = M for every point in Ω .

Exercise 2.3.3 Prove Theorem 2.3.3.

Exercise 2.3.4 Prove Theorem 2.3.1

Corollary Laplace's equation with homogeneous Dirichlet boundary conditions has only the trivial solution u = 0.

From this observation follows the uniqueness of a solution to Poisson's equation with Dirichlet boundary conditions.

Theorem 2.3.4 Let Ω be a bounded region in \mathbb{R}^2 with boundary Γ . Let u satisfy $u = g_0$, $\mathbf{x} \in \Gamma$ and div grad u = f, $\mathbf{x} \in \Omega$. Then u is the only solution to this problem.

Proof. Let *v* be a second solution to the problem. Now consider the difference w = u - v. Clearly w = 0 on Γ and div grad w = 0 on Ω . Hence by the maximum principle $w \equiv 0$ on Ω and u = v.

Theorem 2.3.5 Let u be smooth with continuous second order derivatives, then div grad $u \ge 0$, subject to homogeneous Dirichlet boundary conditions, implies $u \le 0$.

Exercise 2.3.5 *Prove Theorem 2.3.5. Reason by contradiction and follow the proof of Lemma* (2.3.2). \Box

Exercise 2.3.6 Show that the elliptic operator $au_{xx} + 2bu_{xy} + cu_{yy}$, *a,b,c* constant, $ac - b^2 > 0$ satisfies the same maximum principle as the Laplacian operator. Use scaling and rotation of the coordinates.

2.3.3 Existence

To prove *existence* of a solution of Poisson's equation is very hard. In general one needs extra requirements on the smoothness of the boundary. This is far outside the scope of this book, the interested reader may look at [12]. As we shall see in Chapter 7, there is an alternative way to obtain a *generalized* solution to these problems. The existence proof of such a solution is somewhat easier.

2.4 Examples

In this section we give a few examples of PDE's that describe physical and technical problems. For all problems we consider a bounded region $\Omega \subset \mathbb{R}^2$ with boundary Γ .

2.4.1 Flows driven by a potential

Flows driven by a potential we already met in Chapter 1. They all have the form

$$\frac{\partial c(u)}{\partial t} = \operatorname{div} \lambda \,\operatorname{grad} u + f(t, \mathbf{x}, u). \tag{2.4.1}$$

For uniqueness c must be a monotone function of u and for stability it must be nondecreasing. In ordinary heat transfer, ground water flow and diffusion, c is linear. In phase transition problems and diffusion in porous media it is non linear.

2.4.1.1 Boundary conditions

In Section 2.2 there have been introduced three types of boundary conditions that may occur in combination

$$u = g_0(\mathbf{x}), \quad \mathbf{x} \in \Gamma_0, \quad \text{Dirichlet},$$
 (2.4.2a)

$$\lambda \frac{\partial u}{\partial n} = g_1(\mathbf{x}), \quad \mathbf{x} \in \Gamma_1, \quad \text{Neumann},$$
 (2.4.2b)

$$\lambda \frac{\partial u}{\partial n} + \sigma u = g_2(\mathbf{x}), \quad \mathbf{x} \in \Gamma_2, \quad \text{Robbins.}$$
 (2.4.2c)

This is not a limitative enumeration, there are other ways to couple the heat flow at the boundary to the temperature difference one way or another, mostly non linear.

2.4.1.2 Initial condition

In order that Problem 2.4.1 with boundary conditions (2.4.2) has a unique solution $u(\mathbf{x},t)$, it is necessary that u is prescribed at $t = t_0$: $u(\mathbf{x},t_0) = u_0(\mathbf{x}), \forall \mathbf{x} \in \Omega$.

2.4.1.3 Equilibrium

An equilibrium of Equation (2.4.1) is reached when all temporal dependence has disappeared. But this problem can also be considered in its own right:

$$-\operatorname{div} \lambda \operatorname{grad} u = f(\mathbf{x}, u), \qquad (2.4.3)$$

with boundary conditions (2.4.2).

2.4.2 Convection-Diffusion

The *convection-diffusion* equation describes the transport of a pollutant with concentration c by a transporting medium with given velocity **u**. The equation is

$$\frac{\partial c}{\partial t} + \mathbf{u} \cdot \operatorname{grad} c = \operatorname{div} \lambda \, \operatorname{grad} c + f(t, \mathbf{x}, c). \tag{2.4.4}$$

Comparison of Equation (2.4.4) with (2.4.1) shows that a *convection* term $\mathbf{u} \cdot \operatorname{grad} c$ has been added. Boundary and initial conditions are the same as for the potential driven flows.

In cases where the diffusion coefficient λ is small compared to the velocity **u** the flow is *dominated* by the convection. The problem then becomes *singularly perturbed* and in these cases the influence of the second order term is mostly felt at the boundary in the form of *boundary layers*. This causes specific difficulties in the numerical treatment.

2.4.3 Navier-Stokes equations

The Navier-Stokes Equations describe the dynamics of material flow. The momentum equations are given by:

$$\rho(\frac{\partial u}{\partial t} + u\frac{\partial u}{\partial x} + v\frac{\partial u}{\partial y}) = \operatorname{div} \mathbf{s}_x + \rho b_x, \qquad (2.4.5a)$$

$$\rho(\frac{\partial v}{\partial t} + u\frac{\partial v}{\partial x} + v\frac{\partial v}{\partial y}) = \operatorname{div} \mathbf{s}_y + \rho b_y.$$
(2.4.5b)

We shall not derive the equations (see for instance [3]), but we will say a few things about their interpretation. The equations describe Newton's second law on a small volume *V* of fluid with density ρ and velocity $\mathbf{u} = \begin{pmatrix} u \\ v \end{pmatrix}$ moving along with the flow. Thus, a particle $P \in V$ with coordinates \mathbf{x} at time *t* has at time $t + \Delta t$ coordinates $\mathbf{x} + \mathbf{u}\Delta t$. Therefore the change in velocity of a moving particle is described by

$$\Delta \mathbf{u} = \mathbf{u}(\mathbf{x} + \mathbf{u}\Delta t, t + \Delta t) - \mathbf{u}(\mathbf{x}, t).$$
(2.4.6)

We recall Taylors theorem in three variables:

$$f(x+h,y+k,t+\tau) = f(x,y) + h\frac{\partial f}{\partial x} + k\frac{\partial f}{\partial y} + \tau\frac{\partial f}{\partial t} + O(h^2 + k^2 + \tau^2).$$
(2.4.7)

Applying this to Equation (2.4.6) we get:

$$\Delta u = u\Delta t \frac{\partial u}{\partial x} + v\Delta t \frac{\partial u}{\partial y} + \Delta t \frac{\partial u}{\partial t}, \qquad (2.4.8a)$$

$$\Delta v = u\Delta t \frac{\partial v}{\partial x} + v\Delta t \frac{\partial v}{\partial y} + \Delta t \frac{\partial v}{\partial t}.$$
 (2.4.8b)

If we divide both sides by Δt and let $\Delta t \rightarrow 0$ we find the *material derivative*

$$\frac{Du}{Dt} = u\frac{\partial u}{\partial x} + v\frac{\partial u}{\partial y} + \frac{\partial u}{\partial t},$$
(2.4.9a)

$$\frac{Dv}{Dt} = u\frac{\partial v}{\partial x} + v\frac{\partial v}{\partial y} + \frac{\partial v}{\partial t}.$$
(2.4.9b)

The right hand side of Equations (2.4.5) consists of the forces exerted on a (small) volume of fluid. The first term describes surface forces like viscous friction and pressure, the second term describes body forces like gravity. The quantity

$$\Sigma = \begin{pmatrix} \mathbf{s}_{x}^{T} \\ \mathbf{s}_{y}^{T} \end{pmatrix} = \begin{pmatrix} \boldsymbol{\sigma}_{xx} & \boldsymbol{\tau}_{xy} \\ \boldsymbol{\tau}_{yx} & \boldsymbol{\sigma}_{yy} \end{pmatrix}$$
(2.4.10)

is called the stress tensor.

The form of the stress tensor depends on the fluid. A Newtonian fluid has a stress tensor

of the form:

$$\sigma_{xx} = -p + 2\mu \frac{\partial u}{\partial x}, \qquad (2.4.11a)$$

$$\sigma_{yy} = -p + 2\mu \frac{\partial v}{\partial y}, \qquad (2.4.11b)$$

$$\tau_{xy} = \mu(\frac{\partial u}{\partial y} + \frac{\partial v}{\partial x}), \qquad (2.4.11c)$$

in which p is the pressure and μ the viscosity. The minimum configuration to be of practical importance requires a mass conservation equation in addition to (2.4.5):

$$\frac{\partial \rho}{\partial t} + \operatorname{div}(\rho \mathbf{u}) = 0, \qquad (2.4.12)$$

and a functional relation between ρ and p like for instance *Boyle's law*.

An important special case is where ρ is constant and Equation (2.4.12) changes into

$$\operatorname{div} \mathbf{u} = 0, \qquad (2.4.13)$$

the *incompressibility condition*. In this case ρ can be scaled out of Equation (2.4.5) and together with (2.4.11) and (2.4.13) we obtain

$$\frac{\partial u}{\partial t} + u \frac{\partial u}{\partial x} + v \frac{\partial u}{\partial y} + \frac{\partial p}{\partial x} = \mu \Delta u + b_x, \qquad (2.4.14a)$$

$$\frac{\partial v}{\partial t} + u \frac{\partial v}{\partial x} + v \frac{\partial v}{\partial y} + \frac{\partial p}{\partial y} = \mu \Delta v + b_y, \qquad (2.4.14b)$$

$$\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} = 0.$$
 (2.4.14c)

In this case *p* is determined by the equations.

Exercise 2.4.1 Derive Equation (2.4.14).

2.4.3.1 Boundary conditions

On each boundary *two* boundary conditions are needed, a normal and a tangential boundary condition. This can be either the velocity or the stress. The tangential stress is computed by $(\mathbf{t}, \Sigma \cdot \mathbf{n})$ for given unit tangent vector $= \mathbf{t}$ and unit normal vector \mathbf{n} . For an extensive treatment of the Navier-Stokes equations see [37] and [15].

2.4.4 Plane stress

Consider the flat plate in Figure 2.2.

The plate is fixed along side ABC but forces are applied along the free boundary ADB as a consequence of which the plate deforms in the *x*-*y*-plane. We are interested in the stresses $\Sigma = \begin{pmatrix} \sigma_{xx} & \tau_{xy} \\ \tau_{xy} & \sigma_{yy} \end{pmatrix}$ and the *displacements* $\mathbf{u} = \begin{pmatrix} u \\ v \end{pmatrix}$. The differential equations

20

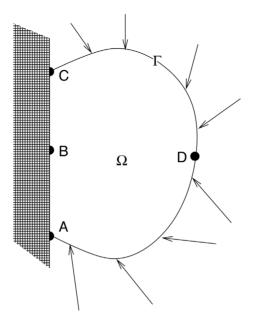


Figure 2.2 Fixed plate with forces applied along the boundary.

for the stresses (compare also (2.4.5)) are given by

$$\frac{\partial \sigma_{xx}}{\partial x} + \frac{\partial \tau_{xy}}{\partial y} + b_1 = 0, \qquad (2.4.15a)$$

$$\frac{\partial \tau_{xy}}{\partial x} + \frac{\partial \sigma_{yy}}{\partial y} + b_2 = 0, \qquad (2.4.15b)$$

in which **b** is the (given) body force per unit volume. Usually only gravity contributes to the body force term. We transform Equations (2.4.15) in two stages into a set of PDE's in the displacements. If the medium is *isotropic* we have a a very simple form of *Hooke's Law* relating stresses and strains:

$$E\varepsilon_x = \sigma_{xx} - v\sigma_{yy}, \qquad (2.4.16a)$$

$$E\varepsilon_{y} = -v\sigma_{xx} + \sigma_{yy}, \qquad (2.4.16b)$$

$$E\gamma_{xy} = \frac{1}{2}(1+\nu)\tau_{xy}.$$
 (2.4.16c)

E, the *modulus of elasticity* and *v*, Poisson's constant, are material constants. Furthermore there is a relation between strain and displacement:

$$\varepsilon_x = \frac{\partial u}{\partial x},$$
 (2.4.17a)

$$\varepsilon_y = \frac{\partial v}{\partial y},$$
 (2.4.17b)

$$\gamma_{xy} = \frac{\partial u}{\partial y} + \frac{\partial v}{\partial x}.$$
 (2.4.17c)

This leads to the following set of PDE's in the displacements **u**:

$$\frac{E}{1-v^2}\frac{\partial}{\partial x}\left(\frac{\partial u}{\partial x}+v\frac{\partial v}{\partial y}\right)+\frac{E}{2(1+v)}\frac{\partial}{\partial y}\left(\frac{\partial u}{\partial y}+\frac{\partial v}{\partial x}\right)=-b_1,$$
(2.4.18a)

$$\frac{E}{2(1+v)}\frac{\partial}{\partial x}\left(\frac{\partial u}{\partial y} + \frac{\partial v}{\partial x}\right) + \frac{E}{1-v^2}\frac{\partial}{\partial y}\left(v\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y}\right) = -b_2.$$
 (2.4.18b)

Exercise 2.4.2 Derive Equations (2.4.18)

2.4.4.1 Boundary conditions

The boundary conditions are comparable to those of the Navier-Stokes equations. At each boundary point we need a normal and a tangential piece of data, either the displacement or the stress.

Exercise 2.4.3 Formulate the boundary conditions along ABC. \square

Exercise 2.4.4 Along ADC the force per unit length is given: **f**. Show that

$$\sigma_{xx}n_x + \tau_{xy}n_y = f_1, \qquad (2.4.19a)$$

$$\tau_{xy}n_x + \sigma_{yy}n_y = f_2, \qquad (2.4.19b)$$

and hence:

$$\frac{n_x E}{1 - v^2} \left(\frac{\partial u}{\partial x} + v \frac{\partial v}{\partial y} \right) + \frac{n_y E}{2(1 + v)} \left(\frac{\partial u}{\partial y} + \frac{\partial v}{\partial x} \right) = f_1, \qquad (2.4.20a)$$

$$\frac{n_x E}{2(1+v)} \left(\frac{\partial u}{\partial y} + \frac{\partial v}{\partial x}\right) + \frac{n_y E}{1-v^2} \left(v\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y}\right) = f_2.$$
(2.4.20b)

2.4.5 Biharmonic equation

The prototype of a fourth order PDE is the biharmonic equation on a bounded region $\Omega \subset \mathbb{R}^2$ with boundary Γ :

$$\Delta \Delta w = f. \tag{2.4.21}$$

It describes the vertical displacement w of a flat plate in the x-y-plane, loaded perpendicularly to that plane. To this problem belong three sets of physical boundary conditions:

1. Clamped boundary

$$w = 0, \quad \frac{\partial w}{\partial n} = 0, \quad \mathbf{x} \in \Gamma.$$
 (2.4.22)

2. Freely supported boundary

$$w = 0, \quad \frac{\partial^2 w}{\partial n^2} + v \frac{\partial^2 w}{\partial t^2} = 0, \quad \mathbf{x} \in \Gamma.$$
 (2.4.23)

3. Free boundary

$$\frac{\partial^2 w}{\partial n^2} + v \frac{\partial^2 w}{\partial t^2} = 0, \quad \frac{\partial^3 w}{\partial n^3} + (2 - v) \frac{\partial^3 w}{\partial t^3} = 0, \quad \mathbf{x} \in \Gamma.$$
(2.4.24)

 $\frac{\partial}{\partial n}$ and $\frac{\partial}{\partial t}$ stand for *normal* and *tangential* derivative respectively. v is Poisson's constant, which depends on the material. In the biharmonic equation the natural boundary conditions contain derivatives of second order or higher, all other boundary conditions are essential.

2.5 Summary of Chapter 2

In this chapter we obtained a classification of second order PDE's into *hyperbolic*, *parabolic* and *elliptic* equations. We formulated appropriate initial and boundary conditions to guarantee a unique solution. We obtained a maximum principle for harmonic functions and used this to prove uniqueness for elliptic equations. We looked at a few examples of partial differential equations in various fields of physics and technology.