

# **Finite Difference Methods for Ordinary and Partial Differential Equations**

# **Finite Difference Methods for Ordinary and Partial Differential Equations**

**Steady-State and Time-Dependent Problems**

**Randall J. LeVeque**

University of Washington  
Seattle, Washington

Copyright © 2007 by the Society for Industrial and Applied Mathematics.

10 9 8 7 6 5 4

All rights reserved. Printed in the United States of America. No part of this book may be reproduced, stored, or transmitted in any manner without the written permission of the publisher. For information, write to the Society for Industrial and Applied Mathematics, 3600 University City Science Center, Philadelphia, PA 19104-2688.

Trademarked names may be used in this book without the inclusion of a trademark symbol. These names are used in an editorial context only; no infringement of trademark is intended.

MATLAB is a registered trademark of The MathWorks, Inc. For MATLAB product information, please contact The MathWorks, Inc., 3 Apple Hill Drive, Natick, MA 01760-2098 USA, 508-647-7000, Fax: 508-647-7101, *info@mathworks.com*, *www.mathworks.com*.

### Library of Congress Cataloging-in-Publication Data

LeVeque, Randall J., 1955-

Finite difference methods for ordinary and partial differential equations : steady-state and time-dependent problems / Randall J. LeVeque.

p.cm.

Includes bibliographical references and index.

ISBN 978-0-898716-29-0 (alk. paper)

1. Finite differences. 2. Differential equations. I. Title.

QA431.L548 2007

515'.35—dc22

2007061732



Partial royalties from the sale of this book are placed in a fund to help students attend SIAM meetings and other SIAM-related activities. This fund is administered by SIAM, and qualified individuals are encouraged to write directly to SIAM for guidelines.

**siam** is a registered trademark.

TO MY FAMILY,  
LOYCE, BEN, BILL, AND ANN

# Contents

<b>Preface</b>	<b>xiii</b>
<b>I Boundary Value Problems and Iterative Methods</b>	<b>1</b>
<b>1 Finite Difference Approximations</b>	<b>3</b>
1.1 Truncation errors . . . . .	5
1.2 Deriving finite difference approximations . . . . .	7
1.3 Second order derivatives . . . . .	8
1.4 Higher order derivatives . . . . .	9
1.5 A general approach to deriving the coefficients . . . . .	10
<b>2 Steady States and Boundary Value Problems</b>	<b>13</b>
2.1 The heat equation . . . . .	13
2.2 Boundary conditions . . . . .	14
2.3 The steady-state problem . . . . .	14
2.4 A simple finite difference method . . . . .	15
2.5 Local truncation error . . . . .	17
2.6 Global error . . . . .	18
2.7 Stability . . . . .	18
2.8 Consistency . . . . .	19
2.9 Convergence . . . . .	19
2.10 Stability in the 2-norm . . . . .	20
2.11 Green's functions and max-norm stability . . . . .	22
2.12 Neumann boundary conditions . . . . .	29
2.13 Existence and uniqueness . . . . .	32
2.14 Ordering the unknowns and equations . . . . .	34
2.15 A general linear second order equation . . . . .	35
2.16 Nonlinear equations . . . . .	37
2.16.1 Discretization of the nonlinear boundary value problem . . . . .	38
2.16.2 Nonuniqueness . . . . .	40
2.16.3 Accuracy on nonlinear equations . . . . .	41
2.17 Singular perturbations and boundary layers . . . . .	43
2.17.1 Interior layers . . . . .	46

2.18	Nonuniform grids . . . . .	49
2.18.1	Adaptive mesh selection . . . . .	51
2.19	Continuation methods . . . . .	52
2.20	Higher order methods . . . . .	52
2.20.1	Fourth order differencing . . . . .	52
2.20.2	Extrapolation methods . . . . .	53
2.20.3	Deferred corrections . . . . .	54
2.21	Spectral methods . . . . .	55
<b>3</b>	<b>Elliptic Equations</b>	<b>59</b>
3.1	Steady-state heat conduction . . . . .	59
3.2	The 5-point stencil for the Laplacian . . . . .	60
3.3	Ordering the unknowns and equations . . . . .	61
3.4	Accuracy and stability . . . . .	63
3.5	The 9-point Laplacian . . . . .	64
3.6	Other elliptic equations . . . . .	66
3.7	Solving the linear system . . . . .	66
3.7.1	Sparse storage in MATLAB . . . . .	68
<b>4</b>	<b>Iterative Methods for Sparse Linear Systems</b>	<b>69</b>
4.1	Jacobi and Gauss–Seidel . . . . .	69
4.2	Analysis of matrix splitting methods . . . . .	71
4.2.1	Rate of convergence . . . . .	74
4.2.2	Successive overrelaxation . . . . .	76
4.3	Descent methods and conjugate gradients . . . . .	78
4.3.1	The method of steepest descent . . . . .	79
4.3.2	The A-conjugate search direction . . . . .	83
4.3.3	The conjugate-gradient algorithm . . . . .	86
4.3.4	Convergence of conjugate gradient . . . . .	88
4.3.5	Preconditioners . . . . .	93
4.3.6	Incomplete Cholesky and ILU preconditioners . . . . .	96
4.4	The Arnoldi process and GMRES algorithm . . . . .	96
4.4.1	Krylov methods based on three term recurrences . . . . .	99
4.4.2	Other applications of Arnoldi . . . . .	100
4.5	Newton–Krylov methods for nonlinear problems . . . . .	101
4.6	Multigrid methods . . . . .	103
4.6.1	Slow convergence of Jacobi . . . . .	103
4.6.2	The multigrid approach . . . . .	106
<b>II</b>	<b>Initial Value Problems</b>	<b>111</b>
<b>5</b>	<b>The Initial Value Problem for Ordinary Differential Equations</b>	<b>113</b>
5.1	Linear ordinary differential equations . . . . .	114
5.1.1	Duhamel’s principle . . . . .	115
5.2	Lipschitz continuity . . . . .	116

5.2.1	Existence and uniqueness of solutions . . . . .	116
5.2.2	Systems of equations . . . . .	117
5.2.3	Significance of the Lipschitz constant . . . . .	118
5.2.4	Limitations . . . . .	119
5.3	Some basic numerical methods . . . . .	120
5.4	Truncation errors . . . . .	121
5.5	One-step errors . . . . .	122
5.6	Taylor series methods . . . . .	123
5.7	Runge–Kutta methods . . . . .	124
5.7.1	Embedded methods and error estimation . . . . .	128
5.8	One-step versus multistep methods . . . . .	130
5.9	Linear multistep methods . . . . .	131
5.9.1	Local truncation error . . . . .	132
5.9.2	Characteristic polynomials . . . . .	133
5.9.3	Starting values . . . . .	134
5.9.4	Predictor-corrector methods . . . . .	135
<b>6</b>	<b>Zero-Stability and Convergence for Initial Value Problems</b>	<b>137</b>
6.1	Convergence . . . . .	137
6.2	The test problem . . . . .	138
6.3	One-step methods . . . . .	138
6.3.1	Euler’s method on linear problems . . . . .	138
6.3.2	Relation to stability for boundary value problems . . . . .	140
6.3.3	Euler’s method on nonlinear problems . . . . .	141
6.3.4	General one-step methods . . . . .	142
6.4	Zero-stability of linear multistep methods . . . . .	143
6.4.1	Solving linear difference equations . . . . .	144
<b>7</b>	<b>Absolute Stability for Ordinary Differential Equations</b>	<b>149</b>
7.1	Unstable computations with a zero-stable method . . . . .	149
7.2	Absolute stability . . . . .	151
7.3	Stability regions for linear multistep methods . . . . .	153
7.4	Systems of ordinary differential equations . . . . .	156
7.4.1	Chemical kinetics . . . . .	157
7.4.2	Linear systems . . . . .	158
7.4.3	Nonlinear systems . . . . .	160
7.5	Practical choice of step size . . . . .	161
7.6	Plotting stability regions . . . . .	162
7.6.1	The boundary locus method for linear multistep methods . . . . .	162
7.6.2	Plotting stability regions of one-step methods . . . . .	163
7.7	Relative stability regions and order stars . . . . .	164
<b>8</b>	<b>Stiff Ordinary Differential Equations</b>	<b>167</b>
8.1	Numerical difficulties . . . . .	168
8.2	Characterizations of stiffness . . . . .	169
8.3	Numerical methods for stiff problems . . . . .	170

8.3.1	A-stability and $A(\alpha)$ -stability . . . . .	171
8.3.2	L-stability . . . . .	171
8.4	BDF methods . . . . .	173
8.5	The TR-BDF2 method . . . . .	175
8.6	Runge–Kutta–Chebyshev explicit methods . . . . .	175
<b>9</b>	<b>Diffusion Equations and Parabolic Problems</b>	<b>181</b>
9.1	Local truncation errors and order of accuracy . . . . .	183
9.2	Method of lines discretizations . . . . .	184
9.3	Stability theory . . . . .	186
9.4	Stiffness of the heat equation . . . . .	186
9.5	Convergence . . . . .	189
9.5.1	PDE versus ODE stability theory . . . . .	191
9.6	Von Neumann analysis . . . . .	192
9.7	Multidimensional problems . . . . .	195
9.8	The locally one-dimensional method . . . . .	197
9.8.1	Boundary conditions . . . . .	198
9.8.2	The alternating direction implicit method . . . . .	199
9.9	Other discretizations . . . . .	200
<b>10</b>	<b>Advection Equations and Hyperbolic Systems</b>	<b>201</b>
10.1	Advection . . . . .	201
10.2	Method of lines discretization . . . . .	203
10.2.1	Forward Euler time discretization . . . . .	204
10.2.2	Leapfrog . . . . .	205
10.2.3	Lax–Friedrichs . . . . .	206
10.3	The Lax–Wendroff method . . . . .	207
10.3.1	Stability analysis . . . . .	209
10.4	Upwind methods . . . . .	210
10.4.1	Stability analysis . . . . .	211
10.4.2	The Beam–Warming method . . . . .	212
10.5	Von Neumann analysis . . . . .	212
10.6	Characteristic tracing and interpolation . . . . .	214
10.7	The Courant–Friedrichs–Lewy condition . . . . .	215
10.8	Some numerical results . . . . .	218
10.9	Modified equations . . . . .	218
10.10	Hyperbolic systems . . . . .	224
10.10.1	Characteristic variables . . . . .	224
10.11	Numerical methods for hyperbolic systems . . . . .	225
10.12	Initial boundary value problems . . . . .	226
10.12.1	Analysis of upwind on the initial boundary value problem	226
10.12.2	Outflow boundary conditions . . . . .	228
10.13	Other discretizations . . . . .	230
<b>11</b>	<b>Mixed Equations</b>	<b>233</b>
11.1	Some examples . . . . .	233



11.2	Fully coupled method of lines . . . . .	235
11.3	Fully coupled Taylor series methods . . . . .	236
11.4	Fractional step methods . . . . .	237
11.5	Implicit-explicit methods . . . . .	239
11.6	Exponential time differencing methods . . . . .	240
11.6.1	Implementing exponential time differencing methods . . . . .	241
<b>III</b>	<b>Appendices</b>	<b>243</b>
<b>A</b>	<b>Measuring Errors</b>	<b>245</b>
A.1	Errors in a scalar value . . . . .	245
A.1.1	Absolute error . . . . .	245
A.1.2	Relative error . . . . .	246
A.2	“Big-oh” and “little-oh” notation . . . . .	247
A.3	Errors in vectors . . . . .	248
A.3.1	Norm equivalence . . . . .	249
A.3.2	Matrix norms . . . . .	250
A.4	Errors in functions . . . . .	250
A.5	Errors in grid functions . . . . .	251
A.5.1	Norm equivalence . . . . .	252
A.6	Estimating errors in numerical solutions . . . . .	254
A.6.1	Estimates from the true solution . . . . .	255
A.6.2	Estimates from a fine-grid solution . . . . .	256
A.6.3	Estimates from coarser solutions . . . . .	256
<b>B</b>	<b>Polynomial Interpolation and Orthogonal Polynomials</b>	<b>259</b>
B.1	The general interpolation problem . . . . .	259
B.2	Polynomial interpolation . . . . .	260
B.2.1	Monomial basis . . . . .	260
B.2.2	Lagrange basis . . . . .	260
B.2.3	Newton form . . . . .	260
B.2.4	Error in polynomial interpolation . . . . .	262
B.3	Orthogonal polynomials . . . . .	262
B.3.1	Legendre polynomials . . . . .	264
B.3.2	Chebyshev polynomials . . . . .	265
<b>C</b>	<b>Eigenvalues and Inner-Product Norms</b>	<b>269</b>
C.1	Similarity transformations . . . . .	270
C.2	Diagonalizable matrices . . . . .	271
C.3	The Jordan canonical form . . . . .	271
C.4	Symmetric and Hermitian matrices . . . . .	273
C.5	Skew-symmetric and skew-Hermitian matrices . . . . .	274
C.6	Normal matrices . . . . .	274
C.7	Toeplitz and circulant matrices . . . . .	275
C.8	The Gershgorin theorem . . . . .	277

C.9	Inner-product norms . . . . .	279
C.10	Other inner-product norms . . . . .	281
<b>D</b>	<b>Matrix Powers and Exponentials</b>	<b>285</b>
D.1	The resolvent . . . . .	286
D.2	Powers of matrices . . . . .	286
	D.2.1 Solving linear difference equations . . . . .	290
	D.2.2 Resolvent estimates . . . . .	291
D.3	Matrix exponentials . . . . .	293
	D.3.1 Solving linear differential equations . . . . .	296
D.4	Nonnormal matrices . . . . .	296
	D.4.1 Matrix powers . . . . .	297
	D.4.2 Matrix exponentials . . . . .	299
D.5	Pseudospectra . . . . .	302
	D.5.1 Nonnormality of a Jordan block . . . . .	304
D.6	Stable families of matrices and the Kreiss matrix theorem . . . . .	304
D.7	Variable coefficient problems . . . . .	307
<b>E</b>	<b>Partial Differential Equations</b>	<b>311</b>
E.1	Classification of differential equations . . . . .	311
	E.1.1 Second order equations . . . . .	311
	E.1.2 Elliptic equations . . . . .	312
	E.1.3 Parabolic equations . . . . .	313
	E.1.4 Hyperbolic equations . . . . .	313
E.2	Derivation of partial differential equations from conservation principles	314
	E.2.1 Advection . . . . .	315
	E.2.2 Diffusion . . . . .	316
	E.2.3 Source terms . . . . .	317
	E.2.4 Reaction-diffusion equations . . . . .	317
E.3	Fourier analysis of linear partial differential equations . . . . .	317
	E.3.1 Fourier transforms . . . . .	318
	E.3.2 The advection equation . . . . .	318
	E.3.3 The heat equation . . . . .	320
	E.3.4 The backward heat equation . . . . .	322
	E.3.5 More general parabolic equations . . . . .	322
	E.3.6 Dispersive waves . . . . .	323
	E.3.7 Even- versus odd-order derivatives . . . . .	324
	E.3.8 The Schrödinger equation . . . . .	324
	E.3.9 The dispersion relation . . . . .	325
	E.3.10 Wave packets . . . . .	327
	<b>Bibliography</b>	<b>329</b>
	<b>Index</b>	<b>337</b>

# Preface

This book evolved from lecture notes developed over the past 20+ years of teaching this material, mostly in Applied Mathematics 585–6 at the University of Washington. The course is taken by first-year graduate students in our department, along with graduate students from mathematics and a variety of science and engineering departments.

Exercises and student projects are an important aspect of any such course and many have been developed in conjunction with this book. Rather than lengthening the text, they are available on the book's Web page:

`www.siam.org/books/OT98`

Along with exercises that provide practice and further exploration of the topics in each chapter, some of the exercises introduce methods, techniques, or more advanced topics not found in the book.

The Web page also contains MATLAB<sup>®</sup> m-files that illustrate how to implement finite difference methods, and that may serve as a starting point for further study of the methods in exercises and projects. A number of the exercises require programming on the part of the student, or require changes to the MATLAB programs provided. Some of these exercises are fairly simple, designed to enable students to observe first hand the behavior of numerical methods described in the text. Others are more open-ended and could form the basis for a course project.

The exercises are available as PDF files. The L<sup>A</sup>T<sub>E</sub>X source is also provided, along with some hints on using L<sup>A</sup>T<sub>E</sub>X for the type of mathematics used in this field. Each exercise is in a separate file so that instructors can easily construct customized homework assignments if desired. Students can also incorporate the source into their solutions if they use L<sup>A</sup>T<sub>E</sub>X to typeset their homework. Personally I encourage this when teaching the class, since this is a good opportunity for them to learn a valuable skill (and also makes grading homework considerably more pleasurable).

## Organization of the Book

The book is organized into two main parts and a set of appendices. Part I deals with steady-state boundary value problems, starting with two-point boundary value problems in one dimension and then elliptic equations in two and three dimensions. Part I concludes with a chapter on iterative methods for large sparse linear systems, with an emphasis on systems arising from finite difference approximations.

Part II concerns time-dependent problems, starting with the initial value problem for ODEs and moving on to initial-boundary value problems for parabolic and hyperbolic PDEs. This part concludes with a chapter on mixed equations combining features of ordinary differential equations (ODEs) and parabolic and hyperbolic equations.

Part III consists of a set of appendices covering background material that is needed at various points in the main text. This material is collected at the end to avoid interrupting the flow of the main text and because many concepts are repeatedly used in different contexts in Parts I and II.

The organization of this book is somewhat different from the way courses are structured at many universities, where a course on ODEs (including both two-point boundary value problems and the initial value problem) is followed by a course on partial differential equations (PDEs) (including both elliptic boundary value problems and time-dependent hyperbolic and parabolic equations). Existing textbooks are well suited to this latter approach, since many books cover numerical methods for ODEs or for PDEs, but often not both. However, I have found over the years that the reorganization into boundary value problems followed by initial value problems works very well. The mathematical techniques are often similar for ODEs and PDEs and depend more on the steady-state versus time-dependent nature of the problem than on the number of dimensions involved. Concepts developed for each type of ODE are naturally extended to PDEs and the interplay between these theories is more clearly elucidated when they are covered together.

At the University of Washington, Parts I and II of this book are used for the second and third quarters of a year-long graduate course. Lectures are supplemented by material from the appendices as needed. The first quarter of the sequence covers direct methods for linear systems, eigenvalue problems, singular values, and so on. This course is currently taught out of Trefethen and Bau [91], which also serves as a useful reference text for the material in this book on linear algebra and iterative methods.

It should also be possible to use this book for a more traditional set of courses, teaching Chapters 1, 5, 6, 7, and 8 in an ODE course followed by Chapters 2, 3, 9, 10, and 11 in a PDE-oriented course.

### **Emphasis of the Book**

The emphasis is on building an understanding of the essential ideas that underlie the development, analysis, and practical use of finite difference methods. Stability theory necessarily plays a large role, and I have attempted to explain several key concepts, their relation to one another, and their practical implications. I include some proofs of convergence in order to motivate the various definitions of “stability” and to show how they relate to error estimates, but have not attempted to rigorously prove all results in complete generality. I have also tried to give an indication of some of the more practical aspects of the algorithms without getting too far into implementation details. My goal is to form a foundation from which students can approach the vast literature on more advanced topics and further explore the theory and/or use of finite difference methods according to their interests and needs.

I am indebted to several generations of students who have worked through earlier versions of this book, found errors and omissions, and forced me to constantly rethink my understanding of this material and the way I present it. I am also grateful to many

colleagues who have taught out of my notes and given me valuable feedback, both at the University of Washington and at more than a dozen other universities where earlier versions have been used in courses. I take full responsibility for the remaining errors.

I have also been influenced by other books covering these same topics, and many excellent ones exist at all levels. Advanced books go into more detail on countless subjects only briefly discussed here, and I give pointers to some of these in the text. There are also a number of general introductory books that may be useful as complements to the presentation found here, including, for example, [27], [40], [49], [72], [84], and [93].

As already mentioned, this book has evolved over the past 20 years. This is true in part for the mundane reason that I have reworked (and perhaps improved) parts of it each time I teach the course. But it is also true for a more exciting reason—the field itself continues to evolve in significant ways. While some of the theory and methods in this book were very well known when I was a student, many of the topics and methods that should now appear in an introductory course had yet to be invented or were in their infancy. I give at least a flavor of some of these, though many other developments have not been mentioned. I hope that students will be inspired to further pursue the study of numerical methods, and perhaps invent even better methods in the future.

*Randall J. LeVeque*