



# Table of Contents

Preface .....	V
---------------	---

<b>A Simple Introduction to Error Estimation for Nonlinear Hyperbolic Conservation Laws</b>	
Bernardo Cockburn .....	1
1 Introduction .....	1
2 Some Convection-Diffusion Problems .....	3
2.1 Traffic Flow .....	4
2.2 Propagation of Phase Transitions .....	8
2.3 Concluding Remarks .....	10
3 Continuous Dependence for Nonlinear Convection-Diffusion .....	10
3.1 The Standard Duality Technique and the Adjoint Problem .....	11
3.2 A Technique to Bypass the Resolution of the Adjoint Problem .....	12
3.3 A Very Simple Way of Handling the Convective Nonlinearity $f$ .....	14
3.4 Continuous Dependence Results in $L^1$ -like Norms .....	16
3.5 Allowing the Diffusion Coefficients to Go to Zero .....	18
3.6 New Continuous Dependence Results .....	21
3.7 Relaxing the Smoothness in Time of the Approximate Solution $u$ .....	24
3.8 The a Posteriori Error Estimate for Non-Smooth $u$ .....	27
3.9 Concluding Remarks .....	28
4 Continuous Dependence for Nonlinear Convection .....	29
4.1 Existence and Uniqueness of the Entropy Solution .....	29
4.2 The Inherited Continuous Dependence Results .....	30
4.3 Concluding Remarks .....	32
5 A Posteriori Error Estimates for Continuous Approximations .....	32
5.1 The Error Estimate .....	32
5.2 Application to the Engquist-Osher Scheme .....	33
5.3 Explaining the Numerical Results .....	34
5.4 Another Error Estimate .....	37
6 A Posteriori Error Estimates for Discontinuous Approximations .....	39
6.1 The Case of a Finite Number of Smooth Discontinuity Curves .....	39
6.2 The Case of a Piecewise-Constant Approximation .....	41

## VIII Table of Contents

7	Concluding Remarks . . . . .	43
7.1	Some Bibliographical Remarks . . . . .	43
7.2	Open Problems . . . . .	43
<b>Notes on Accuracy and Stability of Algorithms in Numerical Linear Algebra</b>		
Nicholas J. Higham . . . . .		47
1	Introduction . . . . .	47
2	Preliminaries . . . . .	47
3	Symmetric Indefinite Systems . . . . .	49
3.1	Block $LDL^T$ Factorization . . . . .	49
3.2	Aasen's Method . . . . .	54
3.3	Aasen's Method Versus Block $LDL^T$ Factorization . . . . .	59
3.4	Tridiagonal Matrices . . . . .	59
4	QR Factorization and Constrained Least Squares Problems . . . . .	60
4.1	Householder QR Factorization . . . . .	61
4.2	The Constrained Least Squares Problem . . . . .	67
5	The Singular Value Decomposition and Jacobi's Method . . . . .	70
5.1	Jacobi's Method . . . . .	71
5.2	Relative Perturbation Theory . . . . .	74
5.3	Error Analysis . . . . .	76
5.4	Other Issues . . . . .	78
<b>Numerical Analysis of Semilinear Parabolic Problems</b>		
Stig Larsson . . . . .		83
1	The Continuous Problem . . . . .	83
2	Local a Priori Error Estimates . . . . .	89
2.1	The Spatially Semidiscrete Problem . . . . .	90
2.2	A Completely Discrete Scheme . . . . .	93
3	Shadowing—First Approach . . . . .	94
3.1	Linearization . . . . .	95
3.2	Exponential Dichotomies . . . . .	98
3.3	Shadowing . . . . .	101
4	A Posteriori Error Estimates . . . . .	105
4.1	The Error Equation . . . . .	106
4.2	Local Estimates of the Residual . . . . .	109
4.3	A Global Error Estimate . . . . .	112
5	Shadowing—Second Approach . . . . .	114
<b>Integration Schemes for Molecular Dynamics and Related Applications</b>		
Robert D. Skeel . . . . .		119
1	Introduction . . . . .	119

2	Newtonian Dynamics . . . . .	121
2.1	Properties . . . . .	121
2.2	The Liouville Equation . . . . .	123
3	The Leapfrog Method . . . . .	125
3.1	Derivation . . . . .	126
3.2	Small- $\Delta t$ Analysis . . . . .	128
3.3	Linear Analysis . . . . .	130
3.4	Small-Energy Analysis . . . . .	132
3.5	Effective Accuracy and Post-Processing . . . . .	134
3.6	Finite-Precision Effects . . . . .	136
4	Other Methods . . . . .	137
4.1	A Family of Methods . . . . .	140
4.2	Quest for Accuracy and Stability . . . . .	141
4.3	The Case for Symplectic Integration . . . . .	143
5	Multiple Time Steps . . . . .	145
5.1	The Verlet-I/r-RESPA/Impulse MTS Method . . . . .	146
5.2	Partitioning of Interactions . . . . .	149
5.3	Efficient Implementation . . . . .	151
5.4	Mollified Impulse MTS Methods . . . . .	152
6	Constrained Dynamics . . . . .	153
6.1	Discretization . . . . .	154
6.2	Solution of the Nonlinear Equations . . . . .	156
7	Constant-Temperature and Constant-Pressure Ensembles . . . . .	156
7.1	Constant-Temperature Ensembles . . . . .	157
7.2	Constant-Pressure Ensembles . . . . .	159
8	Stochastic Dynamics . . . . .	159
8.1	Langevin Dynamics . . . . .	160
8.2	Brownian Dynamics . . . . .	161
A	Lie Series and the BCH Formula . . . . .	162
B	Stochastic Processes . . . . .	164
2.1	Wiener Processes . . . . .	165
2.2	The Ito Integral . . . . .	166
2.3	Stochastic Differential Equations . . . . .	167
2.4	The Fokker–Planck Equation . . . . .	167
2.5	The Ito Formula . . . . .	168
2.6	Weak Ito–Taylor Expansions . . . . .	169
<b>Numerical Methods for Bifurcation Problems</b>		
	Alastair Spence and Ivan G. Graham . . . . .	177
1	Introduction . . . . .	177
2	Examples . . . . .	178
3	Newton’s Method and the Implicit Function Theorem . . . . .	183
3.1	Newton’s Method for Systems . . . . .	183
3.2	The Implicit Function Theorem . . . . .	184

## X Table of Contents

3.3	Two Examples . . . . .	187
4	Computation of Solution Paths . . . . .	188
4.1	Keller's Pseudo-Arclength Continuation [25] . . . . .	189
4.2	Block Elimination . . . . .	192
5	The Computation of Fold (Turning) Points . . . . .	193
5.1	Analysis of Fold Points . . . . .	194
5.2	Numerical Calculation of Fold Points . . . . .	196
6	Bifurcation from the Trivial Solution . . . . .	197
6.1	Scalar Case . . . . .	197
6.2	$n$ -Dimensional Case . . . . .	199
7	Bifurcation in Nonlinear ODEs . . . . .	203
7.1	The Shooting Method for ODEs . . . . .	204
7.2	Analysis of Parameter Dependent ODEs . . . . .	207
7.3	Calculation of Fold Points in ODEs Using Shooting . . . . .	208
8	Hopf Bifurcation . . . . .	209
8.1	Calculation of a Hopf Bifurcation Point . . . . .	210
8.2	The Detection of Hopf Bifurcations in Large Systems . . . . .	212
<b>Spectra and Pseudospectra</b>		
Lloyd N. Trefethen . . . . .		217
1	Eigenvalues . . . . .	217
2	Pseudospectra . . . . .	225
3	A Matrix Example . . . . .	233
4	An Operator Example . . . . .	236
5	History of Pseudospectra . . . . .	243

