# Contents

**Preface**  IX

1  **Definite Integrals**  1  
1.1  Introduction  1  
1.2  Calculation of Weights  2  
1.3  Accuracy of Numerical Methods  3  
1.4  Modification of the Integration Interval  4  
1.5  **Main Integration Methods**  5  
1.5.1  Newton–Cotes Formulae  5  
1.5.2  Gauss Formulae  6  
1.6  **Algorithms Derived from the Trapezoid Method**  9  
1.6.1  Extended Newton–Cotes Formulae  10  
1.6.2  Error in the Extended Formulae  11  
1.6.3  Extrapolation of the Extended Formulae  12  
1.7  Error Control  15  
1.8  Improper Integrals  16  
1.9  Gauss–Kronrod Algorithms  17  
1.10  **Adaptive Methods**  19  
1.10.1  Method Derived from the Gauss–Kronrod Algorithm  20  
1.10.2  Method Derived from the Extended Trapezoid Algorithm  21  
1.10.3  Method Derived from the Gauss–Lobatto Algorithm  22  
1.11  Parallel Computations  23  
1.12  Classes for Definite Integrals  23  
1.13  Case Study: Optimal Adiabatic Bed Reactors for Sulfur Dioxide with Cold Shot Cooling  26  

2  **Ordinary Differential Equations Systems**  31  
2.1  Introduction  31  
2.2  Algorithm Accuracy  35  
2.3  Equation and System Conditioning  36  
2.4  Algorithm Stability  40  
2.5  Stiff Systems  48
2.6 Multistep and Multivalue Algorithms for Stiff Systems 50
2.7 Control of the Integration Step 51
2.8 Runge-Kutta Methods 53
2.9 Explicit Runge-Kutta Methods 54
2.9.1 Strategy to Automatically Control the Integration Step 56
2.9.2 Estimation of the Local Error 58
2.9.2.1 Runge-Kutta-Merson Algorithm 58
2.9.2.2 Richardson Extrapolation 59
2.9.2.3 Embedded Algorithms 59
2.10 Classes Based on Runge-Kutta Algorithms in the BzzMath Library 61
2.11 Semi-Implicit Runge-Kutta Methods 64
2.12 Implicit and Diagonally Implicit Runge-Kutta Methods 66
2.13 Multistep Algorithms 68
2.13.1 Adams-Bashforth Algorithms 70
2.13.2 Adams-Moulton Algorithms 71
2.14 Multivalue Algorithms 72
2.14.1 Control of the Local Error 76
2.14.2 Change the Integration Step 78
2.14.3 Changing the Method Order 79
2.14.4 Strategy for Step and Order Selection 82
2.14.5 Initializing a Multivalue Method 84
2.14.6 Selecting the First Integration Step 84
2.14.7 Selecting the Multivalue Algorithms 84
2.14.7.1 Adams-Moulton Algorithms 85
2.14.7.2 Gear Algorithms 85
2.14.8 Nonlinear System Solution 86
2.15 Multivalue Algorithms for Nonstiff Problems 88
2.16 Multivalue Algorithms for Stiff Problems 90
2.16.1 Robustness in Stiff Problems 93
2.16.1.1 Eigenvalues with a Very Large Imaginary Part 93
2.16.1.2 Problems with Hard Discontinuities 93
2.16.1.3 Variable Constraints 94
2.16.2 Efficiency in Stiff Problems 95
2.16.2.1 When to Factorize the Matrix G 95
2.16.2.2 How to Factorize the Matrix G 96
2.16.2.3 When to Update the Jacobian J 96
2.16.2.4 How to Update the Jacobian J 97
2.17 Multivalue Classes in BzzMath Library 99
2.18 Extrapolation Methods 107
2.19 Some Caveats 108

3 ODE: Case Studies 111
3.1 Introduction 111
3.2 Nonstiff Problems 111
3.3 Volterra System 116
3.4 Simulation of Catalytic Effects 117
3.5 Ozone Decomposition 119
3.6 Robertson's Kinetic 120
3.7 Belousov's Reaction 121
3.8 Fluidized Bed 122
3.9 Problem with Discontinuities 123
3.10 Constrained Problem 124
3.11 Hires Problem 126
3.12 Van der Pol Oscillator 128
3.13 Regression Problems with an ODE Model 129
3.14 Zero-Crossing Problem 139
3.15 Optimization-Crossing Problem 142
3.15.1 Optimization of a Batch Reactor 142
3.15.2 Maximum Level in a Gravity-Flow Tank in Transient Conditions 145
3.15.3 Optimization of a Batch Reactor 148
3.16 Sparse Systems 150
3.17 Use of ODE Systems to Find Steady-State Conditions of Chemical Processes 155
3.18 Industrial Case: Spectrokinetic Modeling 157
3.18.1 CATalytic-Post-Processor 159
3.18.2 Nonreactive CFD Modeling 159
3.18.3 User-Defined Function 160
3.18.4 Reactor Modeling 160
3.18.5 Numerical Methods 162
3.18.6 Dynamic Simulation of an Operando FTIR Cell Used to Study NOx Storage on a LNT Catalyst 163
3.18.7 CAT-PP Simulation Results 166
3.18.8 Nomenclature 169

4 Differential and Algebraic Equation Systems 171
4.1 Introduction 171
4.2 Multivalue Method 174
4.3 DAE Classes in the BzzMath Library 175

5 DAE: Case Studies 187
5.1 Introduction 187
5.2 Van der Pol Oscillator 187
5.3 Regression Problems with the DAE Model 189
5.4 Sparse Structured Matrices 193
5.5 Industrial Case: Distillation Unit 199
5.5.1 Management of System Sparsity and Unstructured Elements 200
5.5.2 DAE Solver for Partially Structured Systems 201