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
2.14.3Changing 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
5.5.3 Case-Study for Solver Validation: Nonequilibrium Distillation
Column Model 202

5.5.4 Numerical Results 205
Notations for Table 5.1 208
Subscripts 208
Symbols 208

6 Boundary Value Problems 209
6.1 Introduction 209
6.1.1 Integral Relationships 211
6.1.2 Continuation Methods 212
6.1.3 Problems with an Unknown Constant Parameter 214
6.1.4 Problem with Unknown Boundary 214
6.2 Shooting Methods 215
6.3 Special Boundary Value Problems 217
6.3.1 Runge–Kutta Implicit Methods 218
6.4 More General BVP Methods 221
6.4.1 Collocation Method 222
6.4.2 Galerkin Method 222
6.4.3 Momentum Method 223
6.4.4 Least-Squares Method 223
6.5 Selection of the Approximating Function 224
6.6 Which and How Many Support Points Have to Be Considered? 225
6.7 Which Variables Should Be Selected as Adaptive Parameters? 231
6.8 The BVP Solution Classes in the BzzMath Library 237
6.9 Adaptive Mesh Selection 251
6.10 Case studies 253

Reference 265

Appendix A: Linking the BzzMath Library to Matlab 269
A.1 Introduction 269
A.2 BzzSum Function 269
A.2.1 Header File 270
A.2.2 MEX Function 270
A.2.3 C++ Part 271
A.2.4 Compiling 272
A.3 Chemical Engineering Example 272
A.3.1 Definition of a New Class 274
A.3.2 Main Program in C++ 275
A.3.3 Main Program in Matlab 277

Appendix B: Copyrights 279

Index 281