

1. Record Nr.	UNINA9910132173103321
Autore	Buzzi-Ferraris G (Guido)
Titolo	Differential and differential-algebraic systems for the chemical engineer : solving numerical problems / / Guido Buzzi-Ferraris and Flavio Manenti
Pubbl/distr/stampa	Weinheim an der Bergstrasse, Germany : , : Wiley-VCH, , 2014 ©2014
ISBN	3-527-66712-1 3-527-66710-5 3-527-66713-X
Descrizione fisica	1 online resource (305 p.)
Disciplina	518.0
Soggetti	Numerical analysis - Data processing Engineering mathematics
Lingua di pubblicazione	Inglese
Formato	Materiale a stampa
Livello bibliografico	Monografia
Note generali	Description based upon print version of record.
Nota di bibliografia	Includes bibliographical references and index.
Nota di contenuto	Differential and Differential-Algebraic Systems for the Chemical Engineer: Solving Numerical Problems; Contents; Preface; 1 Definite Integrals; 1.1 Introduction; 1.2 Calculation of Weights; 1.3 Accuracy of Numerical Methods; 1.4 Modification of the Integration Interval; 1.5 Main Integration Methods; 1.5.1 Newton-Cotes Formulae; 1.5.2 Gauss Formulae; 1.6 Algorithms Derived from the Trapezoid Method; 1.6.1 Extended Newton-Cotes Formulae; 1.6.2 Error in the Extended Formulae; 1.6.3 Extrapolation of the Extended Formulae; 1.7 Error Control; 1.8 Improper Integrals; 1.9 Gauss-Kronrod Algorithms 1.10 Adaptive Methods1.10.1 Method Derived from the Gauss-Kronrod Algorithm; 1.10.2 Method Derived from the Extended Trapezoid Algorithm; 1.10.3 Method Derived from the Gauss-Lobatto Algorithm; 1.11 Parallel Computations; 1.12 Classes for Definite Integrals; 1.13 Case Study: Optimal Adiabatic Bed Reactors for Sulfur Dioxide with Cold Shot Cooling; 2 Ordinary Differential Equations Systems; 2.1 Introduction; 2.2 Algorithm Accuracy; 2.3 Equation and System Conditioning; 2.4 Algorithm Stability; 2.5 Stiff Systems; 2.6 Multistep and Multivalued Algorithms for Stiff Systems

2.7 Control of the Integration Step; 2.8 Runge-Kutta Methods; 2.9 Explicit Runge-Kutta Methods; 2.9.1 Strategy to Automatically Control the Integration Step; 2.9.2 Estimation of the Local Error; 2.9.2.1 Runge-Kutta-Merson Algorithm; 2.9.2.2 Richardson Extrapolation; 2.9.2.3 Embedded Algorithms; 2.10 Classes Based on Runge-Kutta Algorithms in the BzzMath Library; 2.11 Semi-Implicit Runge-Kutta Methods; 2.12 Implicit and Diagonally Implicit Runge-Kutta Methods; 2.13 Multistep Algorithms; 2.13.1 Adams-Bashforth Algorithms; 2.13.2 Adams-Moulton Algorithms; 2.14 Multivalued Algorithms; 2.14.1 Control of the Local Error; 2.14.2 Change the Integration Step; 2.14.3 Changing the Method Order; 2.14.4 Strategy for Step and Order Selection; 2.14.5 Initializing a Multivalued Method; 2.14.6 Selecting the First Integration Step; 2.14.7 Selecting the Multivalued Algorithms; 2.14.7.1 Adams-Moulton Algorithms; 2.14.7.2 Gear Algorithms; 2.14.8 Nonlinear System Solution; 2.15 Multivalued Algorithms for Nonstiff Problems; 2.16 Multivalued Algorithms for Stiff Problems; 2.16.1 Robustness in Stiff Problems; 2.16.1.1 Eigenvalues with a Very Large Imaginary Part; 2.16.1.2 Problems with Hard Discontinuities; 2.16.1.3 Variable Constraints; 2.16.2 Efficiency in Stiff Problems; 2.16.2.1 When to Factorize the Matrix G; 2.16.2.2 How to Factorize the Matrix G; 2.16.2.3 When to Update the Jacobian J; 2.16.2.4 How to Update the Jacobian J; 2.17 Multivalued Classes in BzzMath Library; 2.18 Extrapolation Methods; 2.19 Some Caveats; 3 ODE: Case Studies; 3.1 Introduction; 3.2 Nonstiff Problems; 3.3 Volterra System; 3.4 Simulation of Catalytic Effects; 3.5 Ozone Decomposition; 3.6 Robertson's Kinetic; 3.7 Belousov's Reaction; 3.8 Fluidized Bed; 3.9 Problem with Discontinuities

## Sommario/riassunto

This fourth in a suite of four practical guides is an engineer's companion to using numerical methods for the solution of complex mathematical problems. It explains the theory behind current numerical methods and shows in a step-by-step fashion how to use them. The volume focuses on differential and differential-algebraic systems, providing numerous real-life industrial case studies to illustrate this complex topic. It describes the methods, innovative techniques and strategies that are all implemented in a freely available toolbox called BzzMath, which is developed and maintained by the author.