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Descrizione fisica	1 online resource (XIII, 338 p. 252 illus.)
Collana	Lecture Notes in Physics, , 0075-8450 ; ; 666
Disciplina	541/.37
Soggetti	Physical chemistry Electronics Microelectronics Chemistry, Physical and theoretical Analytical chemistry Computational complexity Chemometrics Physical Chemistry Electronics and Microelectronics, Instrumentation Theoretical and Computational Chemistry Analytical Chemistry Complexity Math. Applications in Chemistry
Lingua di pubblicazione	Inglese
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Note generali	"The book is accompanied (on the webpage http://www.springerlink.com/openurl.asp?genre=journal&issn=1616-6361&volume=666) by a number of example procedures and programs, all in Fortran 90/95"--Pref.
Nota di bibliografia	Includes bibliographical references (p. [313]-329) and index.
Nota di contenuto	Basic Equations -- Approximations to Derivatives -- Ordinary Differential Equations -- The Explicit Method -- Boundary Conditions -- Unequal Intervals -- The Commonly Used Implicit Methods -- Other Methods -- Adsorption -- Effects Due to Uncompensated Resistance and Capacitance -- Two-Dimensional Systems -- Convection -- Performance -- Programming -- Simulation Packages -- Tables and

Formulae -- Some Mathematical Proofs -- Procedure and Program Examples -- References -- Electronic Supplementary Material.

Sommario/riassunto

The book shows how to numerically solve the parabolic partial differential equations (pdes) encountered in electroanalytical chemistry. It does this in a didactic manner, by first introducing the basic equations to be solved and some model systems as text cases, for which solutions exist. Then it treats basic numerical approximation for derivatives and techniques for the numerical solution of ordinary differential equations, from which the more complicated methods for pdes can be derived. The major implicit methods are described in detail, and the handling of homogeneous chemical reactions, including coupled and nonlinear cases, is detailed. More advanced techniques are presented briefly, as well as some commercially available program packages. This third edition, still the only text on the subject, is structured more didactically then the previous editions. It brings the coverage of electrochemical digital simulation up to date, including many new techniques developed since the early 1990s. A number of example procedures and programs are made available as supplementary material in the online version of this book.