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Spectral Methods In Chemistry And Physics Applications To Kinetic Theory And Quantum Mechanics Scientific Computation

Introduction to Spectral Methods for Partial Differential Equations 23.1 - Spectral methods more broadly viewed. Spectral1 Dr Nick Hale - Ultraspherical Spectral Methods Videoconference: The Ultraspherical Spectral Method Leaving the Ivory Tower: Efforts to Bring Spectral Methods of Diagnostics to the Market - Part 1 Spectral4 Yue Lu: \"Spectral Methods for High Dimensional Inference\" Spectral methods for high-dimensional estimation: Asymptotics and fundamental limits Spectral Methods for Matrices and Tensors Spectral Numerical Method Spectral Analysis Talk Jingwei Hu: Deterministic solution of the Boltzmann equation Fast spectral methods

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TRUJILLO GAVIN

Basic Concepts Of Analytical Chemistry

World Scientific
This book presents the fundamental principles, mathematical methods and applications of atmospheric chemistry models for graduate students and researchers.
Advances in Plant Glycosides, Chemistry and Biology R.T. Edwards, Inc.
This book presents the basic algorithms, the main theoretical results, and some applications of spectral methods. Particular attention is paid to the applications of spectral methods to nonlinear problems arising in fluid dynamics, quantum mechanics, weather prediction, heat conduction and other fields.The book consists of three parts. The first part deals with orthogonal approximations in Sobolev spaces and the stability and convergence of approximations for nonlinear problems, as the mathematical foundation of spectral methods. In the second part, various spectral methods are described, with some applications. It includes Fourier spectral method, Legendre spectral method, Chebyshev spectral method, spectral penalty method, spectral vanishing viscosity method, spectral approximation of isolated solutions, multi-dimensional spectral method, spectral method for high-order equations, spectral-domain decomposition method and spectral multigrid method. The third part is devoted to some recent developments of spectral methods, such as mixed spectral methods, combined spectral methods and spectral methods on the surface.

General Analytical Chemistry

Springer Science & Business Media
Numerical Solution of Linear Ordinary Differential Equations in Quantum Chemistry by Spectral Method.
Chemical Analysis Wiley
Chemical Analysis is an essential introduction to a wide range of analytical techniques and instruments. Assuming little in the way of prior knowledge, this text carefully guides the reader through the more widely used and important techniques, whilst avoiding excessive technical detail. Covering both instrumental techniques and the situations in which they are used, the text always strives to maintain a balance between breadth and depth of coverage. Carefully structured, this book clearly differentiates between separation and spectral methods, and includes a section on more specialised techniques. Chemical Analysis * Provides a through introduction to a wide range of the most important and widely used instrumental techniques. * Maintains a careful balance between depth and breadth of coverage. * Includes many examples, problems and their solutions. Chemical Analysis will be invaluable to those studying or using instrumental techniques throughout the sciences, medicine and engineering.

The Alkaloids: Chemistry and Pharmacology

Academic Press
Spectral Methods in Transition Metal Complexes provides a conceptual understanding on how to interpret the optical UV-vis, vibrational EPR, and NMR spectroscopy of transition metal complexes. Metal complexes have broad applications across chemistry in the areas of drug discovery, such as anticancer drugs, sensors, special materials for specific requirements, and catalysis, so a thorough knowledge in preparation and characterization of metal complexes, while niche, is critical. Accessible to both the seasoned researcher and the graduate student alike, this book provides readers with a single source of content that addresses spectral methods in transition metal complexes. Provides readers with a single reference on metal complexes and coordination compounds Contains more than 100 figures, tables, and illustrations to aid in the retention of key concepts Authored by a scientist with nearly 40 years of experience in research and instruction
Mathematical Analysis and Numerical Methods for Science and Technology Elsevier
This is a book about spectral methods for partial differential equations: when to use them, how to implement them, and what can be learned from their of spectral methods has evolved rigorous theory. The computational side vigorously since the early 1970s, especially in computationally intensive of the more spectacular applications are applications in fluid dynamics. Some of the power of these discussed here, first in general terms as examples of the methods have been methods and later in great detail after the specifics covered. This book pays special attention to those algorithmic details which are essential to successful implementation of spectral methods. The focus is on algorithms for fluid dynamical problems in transition, turbulence, and aero dynamics. This book does not address specific applications in meteorology, partly because of the lack of experience of the authors in this field and partly because of the coverage provided by Haltiner and Williams (1980). The success of spectral methods in practical computations has led to an increasing interest in their theoretical aspects, especially since the mid-1970s. Although the theory does not yet cover the complete spectrum of applications, the analytical techniques which have been developed in recent years have facilitated the examination of an increasing number of problems of practical interest. In this book we present a unified theory of the mathematical analysis of spectral methods and apply it to many of the algorithms in current use.
Implementing Spectral Methods for Partial Differential Equations Elsevier
Vibration Fatigue by Spectral Methods relates the structural dynamics theory to the high-cycle vibration fatigue. The book begins with structural dynamics theory and relates the uniaxial and multiaxial vibration fatigue to the underlying structural dynamics and signal processing theory. Organized in two parts, part I gives the theoretical background and part II the selected experimental research. The time- and frequency- domain aspects of signal processing in general, related to structural dynamics and counting methods are covered in detail. It also covers all the underlying theory in structural dynamics, signal processing, uniaxial & multiaxial fatigue; including non-Gaussianity and non-stationarity. Finally, it provides the latest research on multiaxial vibration fatigue and the non-stationarity and non-Gaussianity effects. This book is for engineers, graduate students, researchers and industry professionals working in the field of structural durability under random loading and vibrations and also those dealing with fatigue of materials and constructions. Introduces generalized structural dynamics theory of multiaxial vibration fatigue Maximizes understanding of structural dynamics theory in relation to frequency domain fatigue Illustrates connections between experimental work and theory with case studies, cross-referencing, and parallels to accelerated vibration testing

Spectral Theory of Physical and Chemical Binding: Aspects of Computational Implementation

Academic Press
The broad development of spectroscopy in our country and, in particular, the extensive industrial applications of methods of spectral analysis make the need for basic reference literature a pressing one. Tables of spectral lines, as basic, primary material necessary for the identifica tion of spectra, are the most important of these reference books. The need for such tables is acutely felt by all who work in spectroscopy, and numerous requests for such a book have been received by the Commission on Spectroscopy of the Academy of Sciences of the USSR. On the world book market there are fairly complete tables that cover a very great number of spectral lines and that have been complied rather carefully, although they are not free of errors. Tables of this kind are undoubtedly necessary in general spectroscopic research and must be included among the reference books of large scientific institutions. But the number of workers who need such complete tables is comparatively limited. Therefore, after long discussion it was deemed impractical to republish these tables.
Modeling of Atmospheric Chemistry New Age International
This book provides knowledge of the basic theory, spectral analysis methods, chemometrics, instrumentation, and applications of near-infrared (NIR) spectroscopy—not as a handbook but rather as a sourcebook of NIR spectroscopy. Thus, some emphasis is placed on the description of basic knowledge that is important in learning and using NIR spectroscopy. The book also deals with applications for a variety of research fields that are very useful for a wide range of readers from graduate students to scientists and engineers in both academia and industry. For readers who are novices in NIR spectroscopy, this book provides a good introduction, and for those who already are familiar with the field it affords an excellent means of strengthening their knowledge about NIR spectroscopy and keeping abreast of recent developments.

Spectral Methods And Their Applications

Springer
This book will appeal to both practitioners and researchers in industrial and university analytical laboratories, as well as students specializing in analytical spectroscopy and chemometrics. The subjects covered include the advanced principles of calibration (univariate and multivariate) and the estimation of the peak parameters in spectra with overlapping components. This book differs from existing studies on the subject in that it provides easily reproducible computer calculations

illustrating its significant theoretical statements. As such, it can also serve as a practical guide to lecturers in analytical spectrometry and chemometrics.
Spectral Methods in Transition Metal Complexes Springer Science & Business Media
This book is a pedagogical presentation of the application of spectral and pseudospectral methods to kinetic theory and quantum mechanics. There are additional applications to astrophysics, engineering, biology and many other fields. The main objective of this book is to provide the basic concepts to enable the use of spectral and pseudospectral methods to solve problems in diverse fields of interest and to a wide audience. While spectral methods are generally based on Fourier Series or Chebychev polynomials, non-classical polynomials and associated quadratures are used for many of the applications presented in the book. Fourier series methods are summarized with a discussion of the resolution of the Gibbs phenomenon. Classical and non-classical quadratures are used for the evaluation of integrals in reaction dynamics including nuclear fusion, radial integrals in density functional theory, in elastic scattering theory and other applications. The subject matter includes the calculation of transport coefficients in gases and other gas dynamical problems based on spectral and pseudospectral solutions of the Boltzmann equation. Radiative transfer in astrophysics and atmospheric science, and applications to space physics are discussed. The relaxation of initial non-equilibrium distributions to equilibrium for several different systems is studied with the Boltzmann and Fokker-Planck equations. The eigenvalue spectra of the linear operators in the Boltzmann, Fokker-Planck and Schrödinger equations are studied with spectral and pseudospectral methods based on non-classical orthogonal polynomials. The numerical methods referred to as the Discrete Ordinate Method, Differential Quadrature, the Quadrature Discretization Method, the Discrete Variable Representation, the Lagrange Mesh Method, and others are discussed and compared. MATLAB codes are provided for most of the numerical results reported in the book - see Link under 'Additional Information' on the the right-hand column.

Applications of Numerical Methods in Molecular Spectroscopy

Alpha Science Int'l Ltd.
Progress is reported in the development and implementation of a spectral method for constructing the adiabatic electronic potential energy surfaces of large heterogeneous aggregates of physically or chemically interacting atoms. The work carries forward a program of study initiated some years ago by W. Moffitt to describe aggregate electronic structure solely in terms of the properties of atoms and their pairwise interactions. Necessary and sufficient conditions are described for construction of the transformation from diatomic to spectral-product states, and of the corresponding pair-interaction Hamiltonian matrices required in the development, employing representatives of the diatomic spectral response operator obtained from Fourier expansion of the Coulombic interactions. These conditions help to advance the development of the spectral method as a practical computational tool for electronic structure determinations employing conventional irreducible-symmetry methodology. The approach is illustrated with computational studies of avoided crossings in the potential energy surfaces of small van der Waals bonded NaAr(sub N) aggregates, which serve as useful prototypes for understanding selected attributes of cryogenic high energy density matter (HEDM). An outline is provided of work in progress on general implementation of the spectral method and of its application to cryogenic fuels and oxidizers seeded with trace metals which may exhibit improved combustion performance.
Spectral Methods in Fluid Dynamics Springer
This book deals with the application of spectral methods to problems of uncertainty propagation and quanti?cation in model-based computations. It speci?cally focuses on computational and algorithmic features of these methods which are most useful in dealing with models based on partial differential equations, with special att- tion to models arising in simulations of ?uid ?ows. Implementations are illustrated through applications to elementary problems, as well as more elaborate examples selected from the authors' interests in incompressible vortex-dominated ?ows and compressible ?ows at low Mach numbers. Spectral stochastic methods are probabilistic in nature, and are consequently rooted in the rich mathematical foundation associated with probability and measure spaces. Despite the authors' fascination with this foundation, the discussion only - ludes to those theoretical aspects needed to set the stage for subsequent applications. The book is authored by practitioners, and is primarily intended for researchers or graduate students in computational mathematics, physics, or ?uid dynamics. The book assumes familiarity with elementary methods for the numerical solution of time-dependent, partial differential equations; prior experience with spectral me- ods is naturally helpful though not essential. Full appreciation of elaborate examples in computational ?uid dynamics (CFD) would require familiarity with key, and in some cases delicate, features of the associated numerical methods. Besides these shortcomings, our aim is to treat algorithmic and computational aspects of spectral stochastic methods with details suf?cient to address and reconstruct all but those highly elaborate examples.
Basics of Analytical Chemistry and Chemical Equilibria CRC Press
"The Bisbenzylisoquinoline Alkaloids, reviewed in Vols. 7, 9, 13, and 16 of this treatise, represent the largest group among the isoquinoline alkaloids. Bisbenzylisoquinoline alkaloids tubocurarine, thalicarpine, tetrandrine, and cepharanthine also have interesting pharmacological properties, and for these reasons this group of alkaloids is again updated, covering in the Appendix the pertinent literature until 1985. Indole alkaloids of the rare genus Pauridiantha are presented here for the first time under the title "The Alkaloids from Pauridiantha"; these alkaloids are found almost exclusively in Madagascar, where plant extracts are used by the natives for medicinal purposes. "The Amaryllidaceae Alkaloids," reviewed in Vols. 6, 11, and 15 of this treatise, have been updated, and several new alkaloids of this class are listed. Occurrence, spectral properties, structure, synthesis, and biosynthesis of these alkaloids are covered in these chapters, and pharmacological properties whenever known are reported.
Chebyshev and Fourier Spectral Methods LAP Lambert Academic Publishing
Applications of Numerical Methods in Molecular Spectroscopy provides a mathematical background, theoretical perspective, and review of spectral data processing methods. The book discusses methods of complex spectral profile separation into bands, factor analysis methods, methods of quantitative analysis in molecular spectroscopy and reflectance spectroscopy, and new data processing methods. Mathematical methods in special areas of molecular spectroscopy, such as color science, electron spin resonance, and nuclear magnetic resonance spectroscopies are also covered. The book will benefit researchers and postgraduate students in fields of chemistry, physics, and biology.
Near-Infrared Spectroscopy CRC Press
In the plant kingdom a variety of chemical constituents occur in a glycoside form (conjugation with sugar). Glycosides are important, secondary metabolites. The structural diversity is a result of the vast amount of varieties and stereochemical configurations of the sugar component. Aglycones belong to terpenoid, steroid, flavonoid, quinonoid, lignan, other simple phenolics, and isothiocyanate. However, biological activities of glycosides are, in many cases, susceptible to the nature of sugar moieties, even though their aglycone is the same. Since the 80s, plant glycosides have been attracting an increasing volume of interest from botanists and phytochemists world-wide for the following reasons: • They are difficult to isolate and purify • They have a very important biological function in plant life and remarkable biological activities • They are a very important resource of natural medicine, health food, cosmetics and food supplements. The first International Symposium on Plant Glycosides (ISPG), held in Kunming, China was attended by more than 150 scientists from 17 countries. During the four day meeting, 96 reports on plant glycosides, including structure elucidation, ethnobotany, pharmacology, quantitative evaluation, synthesis, pharmacology and biotechnology were presented. 54 of these papers are given in this volume. All these papers review recent research results on plant glycosides.
Numerical Solution of Linear Ordinary Differential Equations in Quantum Chemistry by Spectral Method
Elsevier
"This volume provides a comprehensive state-of-the-art account, exclusively devoted to the analytical chemistry of Macrocyclic (crown ethers), Macrobicyclic (cryptands) and the Supramolecular compounds (calixarene and calyx(n) resorcinarene and rotaxanes). These compounds having a great deal of similarity in their chemical characteristics have direct application in biosciences, analytical chemistry, solvent extraction, chromatography, spectroscopy and ion selective electrodes."--BOOK JACKET.
Analytical Chemistry of Macrocyclic and Supramolecular Compounds John Wiley & Sons
This book provides key information about the instrumental analytical methods which are the most used in quantitative analysis. A theoretical knowledge of each method is discussed. The methods are illustrated with several examples covering a wide range such as pharmacy, biochemical, environmental and agrochemicals analysis. It is structured into three parts: the first one focuses on separation methods, the second covers the spectroscopic ones and the third part develops the thermal and the radiochemical methods.
Fractional Order Analysis Spectral Methods in Chemistry and Physics
Spectral Methods in Chemistry and PhysicsSpringer
Tables of Spectral Lines Springer
Outlines the basic principles, advanced instrumentation, applications and future potential of a range of spectral techniques in food analysis. The book introduces new applications of GC-MS, LC-MS, MALDI TOF-MS, GC-FTIR, SFC-FTIR, ATR, and Raman spectroscopy. The book covers the identification and quantitation of food constituents, additives and contaminants.