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Spectral Methods In Chemistry And

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.

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Spectral Methods in Chemistry and Physics: Applications to ...

Spectrochemical analysis, methods of chemical analysis that depend upon the measurement of the wavelength and the intensity of electromagnetic radiation. Its major use is in the determination of the arrangement of atoms and electrons in molecules of chemical compounds on the basis of the amounts

chemistry - Encyclopedia Britannica

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.

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Spectral Methods in Chemistry and Physics - MathWorks

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MATLAB Codes - spectralmethods.chem.ubc.ca

Spectroscopy and spectrography are terms used to refer to the measurement of radiation intensity as a function of wavelength and are often used to describe experimental spectroscopic methods. Spectral measurement devices are referred to as spectrometers, spectrophotometers, spectrographs or spectral analyzers.. Daily observations of color can be related to spectroscopy.

Spectroscopy

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Spectral Methods in Chemistry and Physics: Applications to ...

Spectral methods measure the electromagnetic radiation that is absorbed, scattered, or emitted by the analyte. Because the types of radiation that can be monitored are multitudinous and the manner in which the radiation is measured can significantly vary from one method to another, the spectral methods constitute the largest category of instrumental methods.

Chemical analysis - Classical methods | Britannica

Abstract This chapter introduces the basic principles of spectral/pseudospectral methods for the solution of partial differential and/or integral equations that serve to model a large number of physical processes in chemistry and physics.

Introduction to Spectral/Pseudospectral Methods | SpringerLink

A spectrum is defined as the characteristic wavelengths of electromagnetic radiation (or a portion thereof) that is emitted or absorbed by an object or substance, atom, or molecule.

Spectrum Definition in Chemistry - ThoughtCo

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Spectral Methods in Chemistry and Physics: Applications to ...

Since the publication of "Spectral Methods in Fluid Dynamics", spectral methods, particularly in their multidomain version, have become firmly established as a mainstream tool for scientific and engineering computation. While retaining the tight integration between the theoretical and

Spectral Methods - Fundamentals in Single Domains ...

Peak detection is a crucial step in spectral signal pre-processing. The accurate locations of characteristic peaks are prerequisite for chemical identification. However, measured spectra inevitably contain both noise and baseline signals. These interference signals will generate a series of false peaks, which is a challenge for spectral analyses.

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.

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

Completely revised text applies spectral methods to boundary value, eigenvalue, and time-dependent problems, but also covers cardinal functions, matrix-solving methods, coordinate transformations, much more. Includes 7 appendices and over 160 text figures.

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This book contains all advanced spectroscopic methods which are very very essential to identification of a chemical compound. This book will be useful to Master degree students of chemistry, food science, biochemistry etc. The content of this book is designed in such a way that it will be well suited to graduates and post graduate courses of all science disciplines. To carryout the analysis and identification of a new compound.

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.

This book deals with the application of spectral methods to problems of uncertainty propagation and quantification in model-based computations. It specifically focuses on computational and algorithmic features of these methods which are most useful in dealing with models based on partial differential equations, with special attention to models arising in simulations of fluid flows. Implementations are illustrated through applications to elementary problems, as well as more elaborate examples selected from the authors' interests in incompressible vortex-dominated flows and compressible flows 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 alludes 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 fluid dynamics. The book assumes familiarity with elementary methods for the numerical solution of time-dependent, partial differential equations; prior experience with spectral methods is naturally helpful though not essential. Full appreciation of elaborate examples in computational fluid 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 sufficient to address and reconstruct all but those highly elaborate examples.

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.

Along with finite differences and finite elements, spectral methods are one of the three main methodologies for solving partial differential equations on computers. This book provides a detailed presentation of basic spectral algorithms, as well as a systematical presentation of basic convergence theory and error analysis for spectral methods. Readers of this book will be

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Computational
exposed to a unified framework for designing and analyzing spectral algorithms for a variety of problems, including in particular high-order differential equations and problems in unbounded domains. The book contains a large number of figures which are designed to illustrate various concepts stressed in the book. A set of basic matlab codes has been made available online to help the readers to develop their own spectral codes for their specific applications.

Following up the seminal Spectral Methods in Fluid Dynamics, Spectral Methods: Evolution to Complex Geometries and Applications to Fluid Dynamics contains an extensive survey of the essential algorithmic and theoretical aspects of spectral methods for complex geometries. These types of spectral methods were only just emerging at the time the earlier book was published. The discussion of spectral algorithms for linear and nonlinear fluid dynamics stability analyses is greatly expanded. The chapter on spectral algorithms for incompressible flow focuses on algorithms that have proven most useful in practice, has much greater coverage of algorithms for two or more non-periodic directions, and shows how to treat outflow boundaries. Material on spectral methods for compressible flow emphasizes boundary conditions for hyperbolic systems, algorithms for simulation of homogeneous turbulence, and improved methods for shock fitting. This book is a companion to Spectral Methods: Fundamentals in Single Domains.

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