Modeling and Simulation in Science, Engineering and Technology

Modeling and Computational Methods for Kinetic Equations

Pierre Degond Lorenzo Pareschi Giovanni Russo

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reference text or in graduate level courses in kinetic theory and its applications Modeling and Computational Methods for Multi-scale Quantum Dynamics and Kinetic Equations ,2013 This dissertation consists of two parts quantum transitions Part 1 and hydrodynamic limits of kinetic equations Part 2 In both parts we investigate the inner mathematical connections between equations for different physics at different scales and use these connections to design efficient computational methods for multi scale problems Despite its numerous applications in chemistry and physics the mathematics of quantum transition is not well understood Using the Wigner transformation we derive semi classical models in phase space for two problems the dynamics of electrons in crystals near band crossing points surface hopping of quantum molecules when the Born Oppenheimer approximation breaks down In both cases particles may jump between states with comparable energies Our models can capture the transition rates for such processes We provide analytic analysis of and numerical methods for our models demonstrated by explicit examples The second part is to construct numerical methods for kinetic equation that are efficient in the hydrodynamic regime Asymptotically the kinetic equations reduce to fluid dynamics described by the Euler or Navier Stokes equations in the fluid regime Numerically the Boltzmann equation is still hard to handle in the hydrodynamic regime due to the stiff collision term We review the theoretical work that links the two sets of equations and present our asymptotic preserving numerical solvers for the Boltzmann equation that naturally capture the asymptotic limits in the hydrodynamic regime We also extend our methods to the case of multi species systems Modeling Approaches and Computational Methods for Particle-laden Turbulent Flows Shankar Subramaniam, S. Balachandar, 2022-10-20 Modelling Approaches and Computational Methods for Particle laden Turbulent Flows introduces the principal phenomena observed in applications where turbulence in particle laden flow is encountered while also analyzing the main methods for analyzing numerically The book takes a practical approach providing advice on how to select and apply the correct model or tool by drawing on the latest research Sections provide scales of particle laden turbulence and the principal analytical frameworks and computational approaches used to simulate particles in turbulent flow Each chapter opens with a section on fundamental concepts and theory before describing the applications of the modelling approach or numerical method Featuring explanations of key concepts definitions and fundamental physics and equations as well as recent research advances and detailed simulation methods this book is the ideal starting point for students new to this subject as well as an essential reference for experienced researchers Provides a comprehensive introduction to the phenomena of particle laden turbulent flow Explains a wide range of numerical methods including Eulerian Eulerian Lagrange and volume filtered computation Describes a wide range of innovative applications of these models Uncertainty Quantification for Hyperbolic and Kinetic Equations Shi Jin, Lorenzo Pareschi, 2018-03-20 This book explores recent advances in uncertainty quantification for hyperbolic kinetic and related problems The contributions address a range of different aspects including polynomial chaos expansions perturbation methods multi level Monte Carlo methods importance sampling

Advances in Computational Methods in Sciences and Engineering 2005 (2 vols) Theodore Simos, George Maroulis, 2022-05-04 This volume brings together selected contributed papers presented at the International Conference of Computational Methods in Science and Engineering ICCMSE 2005 held in Greece 21 aEURO 26 October 2005 The conference aims to bring together computational scientists from several disciplines in order to share methods and ideas The ICCMSE is unique in its kind It regroups original contributions from all fields of the traditional Sciences Mathematics Physics Chemistry Biology Medicine and all branches of Engineering It would be perhaps more appropriate to define the ICCMSE as a conference on computational science and its applications to science and engineering Topics of general interest are Computational Mathematics Theoretical Physics and Theoretical Chemistry Computational Engineering and Mechanics Computational Biology and Medicine Computational Geosciences and Meteorology Computational Economics and Finance Scientific Computation High Performance Computing Parallel and Distributed Computing Visualization Problem Solving Environments Numerical Algorithms Modelling and Simulation of Complex System Web based Simulation and Computing Grid based Simulation and Computing Fuzzy Logic Hybrid Computational Methods Data Mining Information Retrieval and Virtual Reality Reliable Computing Image Processing Computational Science and Education etc More than 800 extended abstracts have been submitted for consideration for presentation in ICCMSE 2005 From these 500 have been selected after international peer review by at least two independent reviewers Monte Carlo and Ouasi-Monte Carlo Methods Bruno Tuffin, Pierre L'Ecuyer, 2020-05-01 This book presents the refereed proceedings of the 13th International Conference on Monte Carlo and Quasi Monte Carlo Methods in Scientific Computing that was held at the University of Rennes France and organized by Inria in July 2018 These biennial conferences are major events for Monte Carlo and quasi Monte Carlo researchers The proceedings include articles based on invited lectures as well as carefully selected contributed papers on all theoretical aspects and applications of Monte Carlo and quasi Monte Carlo methods Offering information on the latest developments in these very active areas this book is an excellent reference resource for theoreticians and practitioners interested in solving high dimensional computational problems arising in particular in finance statistics and computer graphics **Computational Methods for Polymers** Masoud Soroush,2020-12-10 This book presents recent advances in computational methods for polymers It covers multiscale modeling of polymers polymerization reactions and polymerization

processes as well as control monitoring and estimation methods applied to polymerization processes It presents theoretical insights gained from multiscale modeling validated with exprimental measurements The book consolidates new computational tools and methods developed by academic researchers in this area and presents them systematically The book is useful for graduate students researchers and process engineers and managers **Handbook of Numerical Methods for** Hyperbolic Problems Remi Abgrall, Chi-Wang Shu, 2017-01-16 Handbook on Numerical Methods for Hyperbolic Problems Applied and Modern Issues details the large amount of literature in the design analysis and application of various numerical algorithms for solving hyperbolic equations that has been produced in the last several decades This volume provides concise summaries from experts in different types of algorithms so that readers can find a variety of algorithms under different situations and become familiar with their relative advantages and limitations Provides detailed cutting edge background explanations of existing algorithms and their analysis Presents a method of different algorithms for specific applications and the relative advantages and limitations of different algorithms for engineers or those involved in applications Written by leading subject experts in each field the volumes provide breadth and depth of content coverage Computational Methods in Multiphase Flow V Andrea Alberto Mammoli, C. A. Brebbia, 2009 Together with turbulence multiphase flow remains one of the most challenging areas of computational mechanics and experimental methods and numerous problems remain unsolved to date Multiphase flows are found in all areas of technology at all length scales and flow regimes The fluids involved can be compressible or incompressible linear or nonlinear Because of the complexity of the problems it is often essential to utilize advanced computational and experimental methods to solve the complex equations that describe them Challenges in these simulations include modelling and tracking interfaces dealing with multiple length scales modelling nonlinear fluids treating drop breakup and coalescence characterizing phase structures and many others Experimental techniques although expensive and difficult to perform are essential to validate models This book contains papers presented at the Fifth International Conference on Computational Methods in Multiphase Flow which are grouped into the following topics Multiphase Flow Simulation Interaction of Gas Liquids and Solids Turbulent Flow Environmental Multiphase Flow Bubble and Drop Dynamics Flow in Porous Media Heat Transfer Image Processing Interfacial Behaviour **Implicit-Explicit Methods for** Evolutionary Partial Differential Equations Sebastiano Boscarino, Lorenzo Paresc, Giovanni Russo, 2024-12-12 Implicit explicit IMEX time discretization methods have proven to be highly effective for the numerical solution of a wide class of evolutionary partial differential equations PDEs across various contexts These methods have become mainstream for solving evolutionary PDEs particularly in the fields of hyperbolic and kinetic equations. The first book on the subject Implicit Explicit Methods for Evolutionary Partial Differential Equations provides an in depth yet accessible approach The authors summarize and illustrate the construction analysis and application of IMEX methods using examples test cases and implementation details guide readers through the various methods and teach them how to select and use the one most appropriate for their

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COMPUTATIONAL MODELS - Volume I Shaidurov Vladimir Viktorovich, 2009-04-10 Computational Models is a component of Encyclopedia of Mathematical Sciences in the global Encyclopedia of Life Support Systems EOLSS which is an integrated compendium of twenty one Encyclopedias Modern Computational Mathematics arises in a wide variety of fields including business economics engineering finance medicine and science The Theme on Computational Models provides the essential aspects of Computational Mathematics emphasizing Basic Methods for Solving Equations Numerical Analysis and Methods for Ordinary Differential Equations Numerical Methods and Algorithms Computational Methods and Algorithms

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