Lecture Notes in Computational Science and Engineering



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Hans Petter Langtangen Aslak Tveito Editors

Advanced Topics in Computational Partial Differential Equations

Numerical Methods and Diffpack Programming



Advanced Topics In Computational Partial Differential Equations

Michael Schäfer, Marek Behr, Miriam Mehl, Barbara Wohlmuth

Advanced Topics In Computational Partial Differential Equations:

Advanced Topics in Computational Partial Differential Equations Hans Petter Langtangen, Aslak Tveito, 2003-10-29 A gentle introduction to advanced topics such as parallel computing multigrid methods and special methods for systems of PDEs The goal of all chapters is to compute solutions to problems hence algorithmic and software issues play a central role All software examples use the Diffpack programming environment some experience with Diffpack is required There are also some chapters covering complete applications i e the way from a model expressed as systems of PDEs through to discretization methods algorithms software design verification and computational examples Suitable for readers with a background in basic finite element and finite difference methods for partial differential equations Advanced Topics in Computational Partial Differential Equations Hans Petter Langtangen, Aslak Tveito, 2011-03-30 Advanced Topics in Computational Partial Differential Equations Hans Petter Langtangen, Aslak Tveito, 2012-09-22 This book is about solving partial differential equations PDEs Such equations are used to model a wide range of phenomena in virtually all fields of sci ence and technology Inthe last decade the general availability of extremely powerful computers has shifted the focus in computational mathematics from simplified model problems to much more sophisticated models resembling in tricate features of real life This change challenges our knowledge in computer science and in numerical analysis The main objective of the present book is to teach modern advanced tech niques for numerical PDE solution The book also introduces several models arising in fields likefinance medicine material technology and geology Inor der to read this book you must have a basic knowledge of partial differential equations and numerical methods for solving such equations Furthermore some background in finite element methods is required You do not need to know Diffpack although this programming environment is used in examples throughout the text Basically this book is about models methods and how to implement the methods For the implementation part it is natural for us to use Diffpack as the programming environment because making a PDE solver in Diffpack requires little amount of programming and because Diff pack has support for the advanced numerical methods treated in this book Most chapters have a part on models and methods and a part on imple mentation and Diffpack programming The exposition is designed such that readers can focus only on the first part if desired Computational Partial Differential Equations Hans P. Langtangen, 2012-12-06 The second edition features lots of improvements and new material The most significant additions include finite difference methods and implementations for a 1D time dependent heat equation Chapter 1 7 6 a solver for vibration of elastic structures Chapter 5 1 6 a step by step instruction of how to develop and test Diffpack programs for a physical application Chapters 3 6 and 3 13 construction of non trivial grids using super elements Chapters 3 5 4 3 6 4 and 3 13 4 additional material on local mesh refinements Chapter 3 7 coupling of Diffpack with other types of software Appendix B 3 high level programming offinite difference solvers utilizing the new stencil finite difference operator concept in Diffpack Appendix D 8 Many of the examples projects and exercises from the first edition have

been revised and improved Some new exercises and projects have also been added A hopefully very useful new feature is the compact overview of all the program examples in the book and the associated software files presented in Chapter 1 2 Errors have been corrected many explanations have been extended and the text has been upgraded to be compatible with Diffpack version 4 0 The major difficulty when developing programs for numerical solution of partial differential equations is to debug and verify the implementation This requires an interplay between understanding the mathematical model the in volved numerics and the programming tools Recent Advances in Computational Engineering Michael Schäfer, Marek Behr, Miriam Mehl, Barbara Wohlmuth, 2018-08-21 This book comprises the proceedings of the 4th International Conference on Computational Engineering ICCE 2017 held in Darmstadt Germany on September 28 29 2017 The conference is intended to provide an interdisciplinary meeting place for researchers and practitioners working on computational methods in all disciplines of engineering applied mathematics and computer science The aims of the conference are to discuss the state of the art in this challenging field exchange experiences develop promising perspectives for future research and initiate further cooperation Computational Engineering is a modern and multidisciplinary science for computer based modeling simulation analysis and optimization of complex engineering applications and natural phenomena The book contains an overview of selected approaches from numerics and optimization of Partial Differential Equations as well as uncertainty quantification techniques typically in multiphysics environments Where possible application cases from engineering are integrated The book will be of interest to researchers and practitioners of Computational Engineering Applied Mathematics Engineering Advanced Computational Methods in Science and Engineering Barry Koren, Kees Sciences and Computer Science Vuik, 2010-04-29 The aim of the present book is to show in a broad and yet deep way the state of the art in computational science and engineering Examples of topics addressed are fast and accurate numerical algorithms model order reduction grid computing immersed boundary methods and specific computational methods for simulating a wide variety of challenging problems problems such as fluid structure interaction turbulent flames bone fracture healing micro electro mechanical systems failure of composite materials storm surges particulate flows and so on The main benefit offered to readers of the book is a well balanced up to date overview over the field of computational science and engineering through in depth articles by specialists from the separate disciplines Recent Advances in Algorithmic Differentiation Shaun Forth, Paul Hovland, Eric Phipps, Jean Utke, Andrea Walther, 2012-07-30 The proceedings represent the state of knowledge in the area of algorithmic differentiation AD The 31 contributed papers presented at the AD2012 conference cover the application of AD to many areas in science and engineering as well as aspects of AD theory and its implementation in tools For all papers the referees selected from the program committee and the greater community as well as the editors have emphasized accessibility of the presented ideas also to non AD experts In the AD tools arena new implementations are introduced covering for example Java and graphical modeling environments or join the set of existing tools for Fortran New

developments in AD algorithms target the efficiency of matrix operation derivatives detection and exploitation of sparsity partial separability the treatment of nonsmooth functions and other high level mathematical aspects of the numerical computations to be differentiated Applications stem from the Earth sciences nuclear engineering fluid dynamics and chemistry to name just a few In many cases the applications in a given area of science or engineering share characteristics that require specific approaches to enable AD capabilities or provide an opportunity for efficiency gains in the derivative computation The description of these characteristics and of the techniques for successfully using AD should make the Programming for Computations - Python Svein proceedings a valuable source of information for users of AD tools Linge, Hans Petter Langtangen, 2016-07-25 This book presents computer programming as a key method for solving mathematical problems There are two versions of the book one for MATLAB and one for Python The book was inspired by the Springer book TCSE 6 A Primer on Scientific Programming with Python by Langtangen but the style is more accessible and concise in keeping with the needs of engineering students The book outlines the shortest possible path from no previous experience with programming to a set of skills that allows the students to write simple programs for solving common mathematical problems with numerical methods in engineering and science courses The emphasis is on generic algorithms **Multi-Band Effective Mass** clean design of programs use of functions and automatic tests for verification Approximations Matthias Ehrhardt, Thomas Koprucki, 2014-07-17 This book addresses several mathematical models from the most relevant class of kp Schr dinger systems Both mathematical models and state of the art numerical methods for adequately solving the arising systems of differential equations are presented. The operational principle of modern semiconductor nano structures such as quantum wells quantum wires or quantum dots relies on quantum mechanical effects The goal of numerical simulations using quantum mechanical models in the development of semiconductor nano structures is threefold First they are needed for a deeper understanding of experimental data and of the operational principle Secondly they allow us to predict and optimize in advance the qualitative and quantitative properties of new devices in order to minimize the number of prototypes needed Semiconductor nano structures are embedded as an active region in semiconductor devices Thirdly and finally the results of quantum mechanical simulations of semiconductor nano structures can be used with upscaling methods to deliver parameters needed in semi classical models for semiconductor devices such as quantum well lasers This book covers in detail all these three aspects using a variety of illustrative examples Readers will gain detailed insights into the status of the multiband effective mass method for semiconductor nano structures Both users of the kp method as well as advanced researchers who want to advance the kp method further will find helpful information on how to best work with this method and use it as a tool for characterizing the physical properties of semiconductor nano structures The book is primarily intended for graduate and Ph D students in applied mathematics mathematical physics and theoretical physics as well as all those working in quantum mechanical research or the semiconductor opto electronic

MATLAB Walter Gander, Martin J. Gander, Felix Kwok, 2014-04-23 Scientific computing is the study of how to use computers effectively to solve problems that arise from the mathematical modeling of phenomena in science and engineering It is based on mathematics numerical and symbolic algebraic computations and visualization This book serves as an introduction to both the theory and practice of scientific computing with each chapter presenting the basic algorithms that serve as the workhorses of many scientific codes we explain both the theory behind these algorithms and how they must be implemented in order to work reliably in finite precision arithmetic The book includes many programs written in Matlab and Maple Maple is often used to derive numerical algorithms whereas Matlab is used to implement them The theory is developed in such a way that students can learn by themselves as they work through the text Each chapter contains numerous examples and problems to help readers understand the material hands on

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