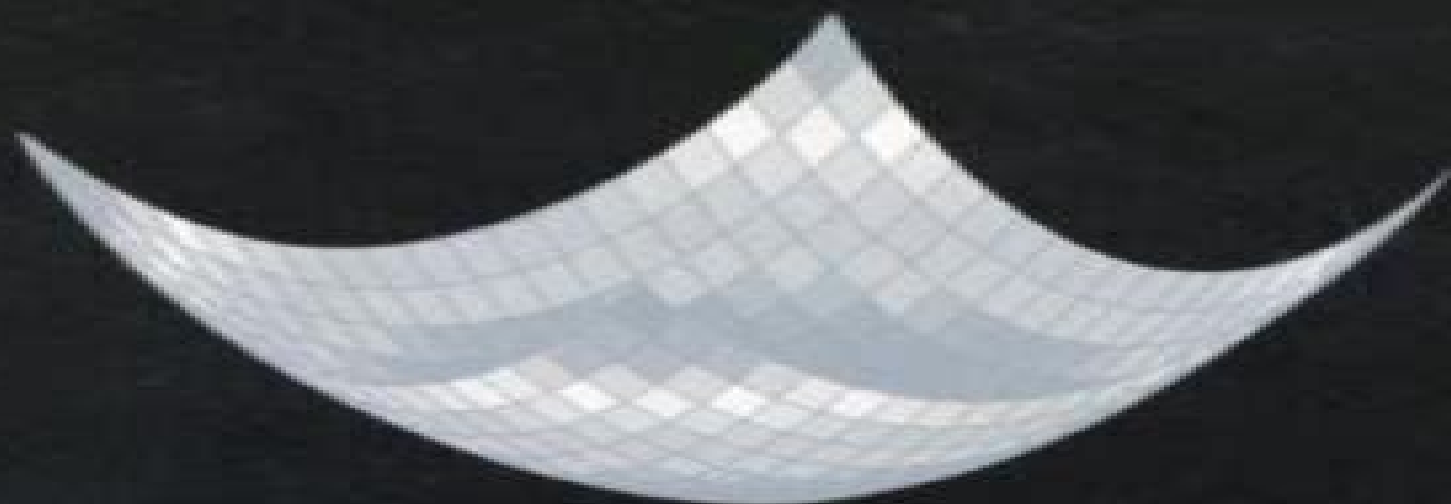


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Accuracy and Reliability in Scientific Computing



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Accuracy And Reliability In Scientific Computing Software Environments Tools

IM Harris



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Accuracy and Reliability in Scientific Computing Bo Einarsson,2005-08-01 This book investigates some of the difficulties related to scientific computing describing how these can be overcome

Introduction to High Performance Scientific Computing David L. Chopp,2019-03-01 Based on a course developed by the author Introduction to High Performance Scientific Computing introduces methods for adding parallelism to numerical methods for solving differential equations It contains exercises and programming projects that facilitate learning as well as examples and discussions based on the C programming language with additional comments for those already familiar with C The text provides an overview of concepts and algorithmic techniques for modern scientific computing and is divided into six self contained parts that can be assembled in any order to create an introductory course using available computer hardware Part I introduces the C programming language for those not already familiar with programming in a compiled language Part II describes parallelism on shared memory architectures using OpenMP Part III details parallelism on computer clusters using MPI for coordinating a computation Part IV demonstrates the use of graphical programming units GPUs to solve problems using the CUDA language for NVIDIA graphics cards Part V addresses programming on GPUs for non NVIDIA graphics cards using the OpenCL framework Finally Part VI contains a brief discussion of numerical methods and applications giving the reader an opportunity to test the methods on typical computing problems

Parallel Processing for Scientific Computing Michael A. Heroux,Padma Raghavan,Horst D. Simon,2006-01-01 Scientific computing has often been called the third approach to scientific discovery emerging as a peer to experimentation and theory Historically the synergy between experimentation and theory has been well understood experiments give insight into possible theories theories inspire experiments experiments reinforce or invalidate theories and so on As scientific computing has evolved to produce results that meet or exceed the quality of experimental and theoretical results it has become indispensable Parallel processing has been an enabling technology in scientific computing for more than 20 years This book is the first in depth discussion of parallel computing in 10 years it reflects the mix of topics that mathematicians computer scientists and computational scientists focus on to make parallel processing effective for scientific problems Presently the impact of parallel processing on scientific computing varies greatly across disciplines but it plays a vital role in most problem domains and is absolutely essential in many of them Parallel Processing for Scientific Computing is divided into four parts The first concerns performance modeling analysis and optimization the second focuses on parallel algorithms and software for an array of problems common to many modeling and simulation applications the third emphasizes tools and environments that can ease and enhance the process of application development and the fourth provides a sampling of applications that require parallel computing for scaling to solve larger and realistic models that can advance science and engineering This edited volume serves as an up to date reference for researchers and application developers on the state of the art in scientific computing It also serves as an excellent overview

and introduction especially for graduate and senior level undergraduate students interested in computational modeling and simulation and related computer science and applied mathematics aspects Contents List of Figures List of Tables Preface Chapter 1 Frontiers of Scientific Computing An Overview Part I Performance Modeling Analysis and Optimization Chapter 2 Performance Analysis From Art to Science Chapter 3 Approaches to Architecture Aware Parallel Scientific Computation Chapter 4 Achieving High Performance on the BlueGene L Supercomputer Chapter 5 Performance Evaluation and Modeling of Ultra Scale Systems Part II Parallel Algorithms and Enabling Technologies Chapter 6 Partitioning and Load Balancing Chapter 7 Combinatorial Parallel and Scientific Computing Chapter 8 Parallel Adaptive Mesh Refinement Chapter 9 Parallel Sparse Solvers Preconditioners and Their Applications Chapter 10 A Survey of Parallelization Techniques for Multigrid Solvers Chapter 11 Fault Tolerance in Large Scale Scientific Computing Part III Tools and Frameworks for Parallel Applications Chapter 12 Parallel Tools and Environments A Survey Chapter 13 Parallel Linear Algebra Software Chapter 14 High Performance Component Software Systems Chapter 15 Integrating Component Based Scientific Computing Software Part IV Applications of Parallel Computing Chapter 16 Parallel Algorithms for PDE Constrained Optimization Chapter 17 Massively Parallel Mixed Integer Programming Chapter 18 Parallel Methods and Software for Multicomponent Simulations Chapter 19 Parallel Computational Biology Chapter 20 Opportunities and Challenges for Parallel Computing in Science and Engineering Index

PETSc for Partial Differential Equations: Numerical Solutions in C and Python Ed

Bueler,2020-10-22 The Portable Extensible Toolkit for Scientific Computation PETSc is an open source library of advanced data structures and methods for solving linear and nonlinear equations and for managing discretizations This book uses these modern numerical tools to demonstrate how to solve nonlinear partial differential equations PDEs in parallel It starts from key mathematical concepts such as Krylov space methods preconditioning multigrid and Newton s method In PETSc these components are composed at run time into fast solvers Discretizations are introduced from the beginning with an emphasis on finite difference and finite element methodologies The example C programs of the first 12 chapters listed on the inside front cover solve mostly elliptic and parabolic PDE problems Discretization leads to large sparse and generally nonlinear systems of algebraic equations For such problems mathematical solver concepts are explained and illustrated through the examples with sufficient context to speed further development PETSc for Partial Differential Equations addresses both discretizations and fast solvers for PDEs emphasizing practice more than theory Well structured examples lead to run time choices that result in high solver performance and parallel scalability The last two chapters build on the reader s understanding of fast solver concepts when applying the Firedrake Python finite element solver library This textbook the first to cover PETSc programming for nonlinear PDEs provides an on ramp for graduate students and researchers to a major area of high performance computing for science and engineering It is suitable as a supplement for courses in scientific computing or numerical methods for differential equations

Spectral Methods in MATLAB Lloyd N. Trefethen,2000-01-01 This is

the only book on spectral methods built around MATLAB programs Along with finite differences and finite elements spectral methods are one of the three main technologies for solving partial differential equations on computers Since spectral methods involve significant linear algebra and graphics they are very suitable for the high level programming of MATLAB This hands on introduction is built around forty short and powerful MATLAB programs which the reader can download from the World Wide Web The Art of Differentiating Computer Programs Uwe Naumann,2012-01-01 This is the first entry level book on algorithmic also known as automatic differentiation AD providing fundamental rules for the generation of first and higher order tangent linear and adjoint code The author covers the mathematical underpinnings as well as how to apply these observations to real world numerical simulation programs Readers will find examples and exercises including hints to solutions the prototype AD tools dco and dcc for use with the examples and exercises first and higher order tangent linear and adjoint modes for a limited subset of C C provided by the derivative code compiler dcc a supplementary website containing sources of all software discussed in the book additional exercises and comments on their solutions growing over the coming years links to other sites on AD and errata

Performance Optimization of Numerically Intensive Codes Stefan Goedecker,Adolfy Hoesie,2001-01-01 Performance Optimization of Numerically Intensive Codes offers a comprehensive tutorial style hands on introductory and intermediate level treatment of all the essential ingredients for achieving high performance in numerical computations on modern computers The authors explain computer architectures data traffic and issues related to performance of serial and parallel code optimization exemplified by actual programs written for algorithms of wide interest The unique hands on style is achieved by extensive case studies using realistic computational problems The performance gain obtained by applying the techniques described in this book can be very significant The book bridges the gap between the literature in system architecture the one in numerical methods and the occasional descriptions of optimization topics in computer vendors literature It also allows readers to better judge the suitability of certain computer architecture to their computational requirements In contrast to standard textbooks on computer architecture and on programming techniques the book treats these topics together at the level necessary for writing high performance programs The book facilitates easy access to these topics for computational scientists and engineers mainly interested in practical issues related to efficient code development

Automatic Differentiation in MATLAB Using ADMAT with Applications Thomas F. Coleman,Wei Xu,2016-06-20 The calculation of partial derivatives is a fundamental need in scientific computing Automatic differentiation AD can be applied straightforwardly to obtain all necessary partial derivatives usually first and possibly second derivatives regardless of a code s complexity However the space and time efficiency of AD can be dramatically improved sometimes transforming a problem from intractable to highly feasible if inherent problem structure is used to apply AD in a judicious manner Automatic Differentiation in MATLAB using ADMAT with Applications discusses the efficient use of AD to solve real problems especially multidimensional zero finding and optimization in the MATLAB

environment This book is concerned with the determination of the first and second derivatives in the context of solving scientific computing problems with an emphasis on optimization and solutions to nonlinear systems The authors focus on the application rather than the implementation of AD solve real nonlinear problems with high performance by exploiting the problem structure in the application of AD and provide many easy to understand applications examples and MATLAB templates

Numerically Solving Polynomial Systems with Bertini Daniel J. Bates,Jonathan D. Hauenstein,Andrew J. Sommese,Charles W. Wampler,2013-11-08 This book is a guide to concepts and practice in numerical algebraic geometry the solution of systems of polynomial equations by numerical methods Through numerous examples the authors show how to apply the well received and widely used open source Bertini software package to compute solutions including a detailed manual on syntax and usage options The authors also maintain a complementary web page where readers can find supplementary materials and Bertini input files Numerically Solving Polynomial Systems with Bertini approaches numerical algebraic geometry from a user s point of view with numerous examples of how Bertini is applicable to polynomial systems It treats the fundamental task of solving a given polynomial system and describes the latest advances in the field including algorithms for intersecting and projecting algebraic sets methods for treating singular sets the nascent field of real numerical algebraic geometry and applications to large polynomial systems arising from differential equations Those who wish to solve polynomial systems can start gently by finding isolated solutions to small systems advance rapidly to using algorithms for finding positive dimensional solution sets curves surfaces etc and learn how to use parallel computers on large problems These techniques are of interest to engineers and scientists in fields where polynomial equations arise including robotics control theory economics physics numerical PDEs and computational chemistry

A Software Repository for Orthogonal Polynomials Walter Gautschi,2018-03-20 A Software Repository for Orthogonal Polynomials is the first book that provides graphs and references to online datasets that enable the generation of a large number of orthogonal polynomials with classical quasi classical and nonclassical weight functions Useful numerical tables are also included The book will be of interest to scientists engineers applied mathematicians and statisticians

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