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Content Description #Includes bibliographical references and index.
Building upon the wide-ranging success of the first edition, Parallel Scientific Computation presents a single unified approach to using a range of parallel computers, from a small desktop computer to a massively parallel computer. The author explains how to use the bulk synchronous parallel (BSP) model to design and implement parallel algorithms in the areas of scientific computing and big data, and provides a full treatment of core problems in these areas, starting from a high-level problem description, via a sequential solution algorithm to a parallel solution algorithm and an actual parallel program written in BSPlib. Every chapter of the book contains a theoretical section and a practical section presenting a parallel program and numerical experiments on a modern parallel computer to put the theoretical predictions and cost analysis to the test. Every chapter also presents extensive bibliographical notes with additional discussions and pointers to relevant literature, and numerous exercises which are suitable as graduate student pro-

jects. The second edition provides new material relevant for big-data science such as sorting and graph algorithms, and it provides a BSP approach towards new hardware developments such as hierarchical architectures with both shared and distributed memory. A single, simple hybrid BSP system suffices to handle both types of parallelism efficiently, and there is no need to master two systems, as often happens in alternative approaches. Furthermore, the second edition brings all algorithms used up to date, and it includes new material on high-performance linear system solving by LU decomposition, and improved data partitioning for sparse matrix computations. The book is accompanied by a software package BSPedupack, freely available online from the author's homepage, which contains all programs of the book and a set of test driver programs. This package written in C can be run using modern BSPlib implementations such as MulticoreBSP for C or BSPonMPI.

Numerical software is used to test scientific theories, design airplanes and bridges, operate manufacturing lines, control power plants and refineries, analyze financial derivatives, identify genomes, and provide the understanding necessary to derive and analyze cancer treatments. Because of the high stakes involved, it is essential that results computed using software be accurate, reliable, and robust. Unfortunately, developing accurate and reliable scientific software is notoriously difficult. This book investigates some of the difficulties related to scientific computing and provides insight into how to overcome them and obtain dependable results. The tools to assess existing scientific applications are described, and a variety of techniques that can improve the accuracy and reliability of newly developed applications is discussed. Accuracy and Reliability in Scientific Computing can be considered a handbook for improving the quality of scientific computing. It will help computer scientists address the problems that affect software in general as well as the particular challenges of numerical computation: approximations occurring at all levels, continuous functions replaced by discretized versions, infinite processes replaced by finite ones, and real numbers replaced by finite precision numbers. Divided into three parts, it starts by illustrating some of the difficulties in producing robust and reliable scientific software. Well-known cases of failure are reviewed and the what and why of numerical computations are considered. The second section describes diagnostic tools that can be used to assess the accuracy and reliability of existing scientific applications. In the last section, the authors describe a variety of techniques that can be employed to improve the accuracy and reliability of newly developed scientific applications. The authors of the individual chapters are international experts, many of them members of the IFIP Working Group on Numerical Software.

Foreword by Bjarne Stroustrup Software is generally acknowledged to be the single greatest obstacle preventing mainstream adoption of massively-parallel computing. While sequential applications are routinely ported to platforms ranging from PCs to mainframes, most parallel programs only ever run on one type of machine. One reason for this is that most parallel programming systems have failed to insulate their users from the architectures of the machines on which

they have run. Those that have been platform-independent have usually also had poor performance. Many researchers now believe that object-oriented languages may offer a solution. By hiding the architecture-specific constructs required for high performance inside platform-independent abstractions, parallel object-oriented programming systems may be able to combine the speed of massively--parallel computing with the comfort of sequential programming. Parallel Programming Using C++ describes fifteen parallel programming systems based on C++, the most popular object-oriented language of today. These systems cover the whole spectrum of parallel programming paradigms, from data parallelism through dataflow and distributed shared memory to message-passing control parallelism. For the parallel programming community, a common parallel application is discussed in each chapter, as part of the description of the system itself. By comparing the implementations of the polygon overlay problem in each system, the reader can get a better sense of their expressiveness and functionality for a common problem. For the systems community, the chapters contain a discussion of the implementation of the various compilers and runtime systems. In addition to discussing the performance of polygon overlay, several of the contributors also discuss the performance of other, more substantial, applications. For the research community, the contributors discuss the motivations for and philosophy of their systems. As well, many of the chapters include critiques that complete the research arc by pointing out possible future research directions. Finally, for the object-oriented community, there are many examples of how encapsulation, inheritance, and polymorphism can be used to control the complexity of developing, debugging, and tuning parallel software.

Combinatorial Scientific Computing explores the latest research on creating algorithms and software tools to solve key combinatorial problems on large-scale high-performance computing architectures. It includes contributions from international researchers who are pioneers in designing software and applications for high-performance computing systems

This book constitutes the refereed proceedings of the Third International Symposium on Computing in Object-Oriented Parallel Environments, ISCOPE 99, held in San Francisco, CA, USA in December 1999. The 14 revised full papers presented together with six short papers were selected from 41 submissions. The papers are devoted to compilers and optimization techniques, new application fields, components and metacomputing, numerical frameworks, generic programming and skeletons, application-specific frameworks, and runtime systems and techniques.

This is the first text explaining how to use the bulk synchronous parallel (BSP) model and the freely available BSPlib communication library in parallel algorithm design and parallel programming. Aimed at graduate students and researchers in mathematics, physics and computer science, the main topics treated in the book are core topics in the area of scientific computation and many additional topics are treated in numerous exercises. An appendix on the message-passing interface (MPI) discusses how to program using the MPI communication library. MPI equivalents of all the programs are also present-

ed. The main topics treated in the book are core in the area of scientific computation: solving dense linear systems by Gaussian elimination, computing fast Fourier transforms, and solving sparse linear systems by iterative methods. Each topic is treated in depth, starting from the problem formulation and a sequential algorithm, through a parallel algorithm and its analysis, to a complete parallel program written in C and BSPlib, and experimental results obtained using this program on a parallel computer. Additional topics treated in the exercises include: data compression, random number generation, cryptography, eigensystem solving, 3D and Strassen matrix multiplication, wavelets and image compression, fast cosine transform, decimals of pi, simulated annealing, and molecular dynamics. The book contains five small but complete example programs written in BSPlib which illustrate the methods taught. The appendix on MPI discusses how to program in a structured, bulk synchronous parallel style using the MPI communication library. It presents MPI equivalents of all the programs in the book. The complete programs of the book and their driver programs are freely available online in the packages BSPedupack and MPIedupack.

This easy-to-read textbook/reference presents an essential guide to object-oriented C++ programming for scientific computing. With a practical focus on learning by example, the theory is supported by numerous exercises. Features: provides a specific focus on the application of C++ to scientific computing, including parallel computing using MPI; stresses the importance of a clear programming style to minimize the introduction of errors into code; presents a practical introduction to procedural programming in C++, covering variables, flow of control, input and output, pointers, functions, and reference variables; exhibits the efficacy of classes, highlighting the main features of object-orientation; examines more advanced C++ features, such as templates and exceptions; supplies useful tips and examples throughout the text, together with chapter-ending exercises, and code available to download from Springer.

In modern computer science, there exists no truly sequential computing system; and most advanced programming is parallel programming. This is particularly evident in modern application domains like scientific computation, data science, machine intelligence, etc. This lucid introductory textbook will be invaluable to students of computer science and technology, acting as a self-contained primer to parallel programming. It takes the reader from introduction to expertise, addressing a broad gamut of issues. It covers different parallel programming styles, describes parallel architecture, includes parallel programming frameworks and techniques, presents algorithmic and analysis techniques and discusses parallel design and performance issues. With its broad coverage, the book can be useful in a wide range of courses; and can also prove useful as a ready reckoner for professionals in the field.

This book presents the state of the art in parallel numerical algorithms, applications, architectures, and system software. The book examines various solutions for issues of concurrency, scale, energy efficiency, and programmability, which are discussed in the context of a diverse range of appli-

cations. Features: includes contributions from an international selection of world-class authorities; examines parallel algorithm-architecture interaction through issues of computational capacity-based codesign and automatic restructuring of programs using compilation techniques; reviews emerging applications of numerical methods in information retrieval and data mining; discusses the latest issues in dense and sparse matrix computations for modern high-performance systems, multicores, manycores and GPUs, and several perspectives on the Spike family of algorithms for solving linear systems; presents outstanding challenges and developing technologies, and puts these in their historical context.

The Numerical Recipes Code CD -ROM contains, in a single omnibus edition, all the source code for the routines and examples from: Numerical Recipes in Fortran 77: The Art of Scientific Computing (Second Edition), Numerical Recipes in Fortran 90: The Art of Parallel Scientific Computing, Numerical Recipes in C: The Art of Scientific Computing (Second Edition), both ANSI and K&R C, Numerical Recipes in Pascal: The Art of Scientific Computing,and Numerical Recipes Routines and Examples in BASIC. The ISO 9660 standard format CD-ROM includes HTML files that allow the use of any Web browser to navigate among all the program files. The CD-ROM also contains the complete public domain SLATEC Common Mathematical Library, a comprehensive collection of over 1400 mathematical and statistical routines. A UNIX one-screen code use license is included.

Created to help scientists and engineers write computer code, this practical book addresses the important tools and techniques that are necessary for scientific computing, but which are not yet commonplace in science and engineering curricula. This book contains chapters summarizing the most important topics that computational researchers need to know about. It leverages the viewpoints of passionate experts involved with scientific computing courses around the globe and aims to be a starting point for new computational scientists and a reference for the experienced. Each contributed chapter focuses on a specific tool or skill, providing the content needed to provide a working knowledge of the topic in about one day. While many individual books on specific computing topics exist, none is explicitly focused on getting technical professionals and students up and running immediately across a variety of computational areas.

Accompanying CD-ROM has a software suite containing all the functions and programs discussed.

The purpose of this book is to survey some recent advances in the development of software tools for scientific computing. This book presents 17 carefully selected and refereed chapters originally presented at the SciTools '96 Workshop in Oslo, Norway. The chapters emphasize the design of large software codes, computational efficiency, object-oriented programming in scientific computing, reliability of numerical software, and parallel computing.

This simple-to-follow textbook/reference provides an invaluable guide to object-oriented C++ programming for scientific computing. Through a series of clear and concise discussions, the key features most useful to the novice programmer are explored, enabling the reader to quickly master

the basics and build the confidence to investigate less well-used features when needed. The text presents a hands-on approach that emphasizes the benefits of learning by example, stressing the importance of a clear programming style to minimise the introduction of errors into the code, and offering an extensive selection of practice exercises. This updated and enhanced new edition includes additional material on software testing, and on some new features introduced in modern C++ standards such as C++11. Topics and features: presents a practical treatment of the C++ programming language for applications in scientific computing; reviews the essentials of procedural programming in C++, covering variables, flow of control, input and output, pointers, functions and reference variables; introduces the concept of classes, showcasing the main features of object-orientation, and discusses such advanced C++ features as templates and exceptions; examines the development of a collection of classes for linear algebra calculations, and presents an introduction to parallel computing using MPI; describes how to construct an object-oriented library for solving second order differential equations; contains appendices reviewing linear algebra and useful programming constructs, together with solutions to selected exercises; provides exercises and programming tips at the end of every chapter, and supporting code at an associated website. This accessible textbook is a "must-read" for programmers of all levels of expertise. Basic familiarity with concepts such as operations between vectors and matrices, and the Newton-Raphson method for finding the roots of non-linear equations, would be an advantage, but extensive knowledge of the underlying mathematics is not assumed.

Science used to be experiments and theory, now it is experiments, theory and computations. The computational approach to understanding nature and technology is currently flowering in many fields such as physics, geophysics, astrophysics, chemistry, biology, and most engineering disciplines. This book is a gentle introduction to such computational methods where the techniques are explained through examples. It is our goal to teach principles and ideas that carry over from field to field. You will learn basic methods and how to implement them. In order to gain the most from this text, you will need prior knowledge of calculus, basic linear algebra and elementary programming.

This is the greatly revised and greatly expanded Second Edition of the hugely popular Numerical Recipes: The Art of Scientific Computing. The product of a unique collaboration among four leading scientists in academic research and industry Numerical Recipes is a complete text and reference book on scientific computing. In a self-contained manner it proceeds from mathematical and theoretical considerations to actual practical computer routines. With over 100 new routines bringing the total to well over 300, plus upgraded versions of the original routines, this new edition remains the most practical, comprehensive handbook of scientific computing available today. Highlights of the new material include: -A new chapter on integral equations and inverse methods -Multigrid and other methods for solving partial differential equations -Improved random number routines -

Wavelet transforms -The statistical bootstrap method -A new chapter on "less-numerical" algorithms including compression coding and arbitrary precision arithmetic. The book retains the informal easy-to-read style that made the first edition so popular, while introducing some more advanced topics. It is an ideal textbook for scientists and engineers and an indispensable reference for anyone who works in scientific computing. The Second Edition is availabe in FORTRAN, the traditional language for numerical calculations and in the increasingly popular C language.

It is the combination of mathematical ideas and efficient programs that drives the progress in many scientific disciplines: The faster results can be generated on a computer, the bigger and the more accurate are the challenges that can be solved. This textbook targets students who have programming skills and do not shy away from mathematics, though they might be educated in computer science or an application domain and have no primary interest in the maths. The book is for students who want to see some simulations up and running. It introduces the basic concepts and ideas behind applied mathematics and parallel programming that are needed to write numerical simulations for todays multicore workstations. The intention is not to dive into one particular application domain or to introduce a new programming language; rather it is to lay the generic foundations for future studies and projects in this field. Topics and features: Fits into many degrees where students have already been exposed to programming languages Pairs an introduction to mathematical concepts with an introduction to parallel programming Emphasises the paradigms and ideas behind code parallelisation, so students can later on transfer their knowledge and skills Illustrates fundamental numerical concepts, preparing students for more formal textbooks The easily digestible text prioritises clarity and intuition over formalism, illustrating basic ideas that are of relevance in various subdomains of scientific computing. Its primary goal is to make theoretical and paradigmatic ideas accessible and even fascinating to undergraduate students. Tobias Weinzierl is professor in the Department of Computer Science at Durham University, Durham, UK. He has worked at the Munich Centre for Advanced Computing (see the Springer edited book, Advanced Computing) before, and holds a PhD and habilitation from the Technical University Munich.

Here, authors from academia and practice provide practitioners, scientists and graduates with basic methods and paradigms, as well as important issues and trends across the spectrum of parallel and distributed processing. In particular, they cover such fundamental topics as efficient parallel algorithms, languages for parallel processing, parallel operating systems, architecture of parallel and distributed systems, management of resources, tools for parallel computing, parallel database systems and multimedia object servers, as well as the relevant networking aspects. A chapter is dedicated to each of parallel and distributed scientific computing, high-performance computing in molecular sciences, and multimedia applications for parallel and distributed systems.

This is a textbook that teaches the bridging topics between numerical analysis, parallel comput-

ing, code performance, large scale applications.

Architecture-independent programming and automatic parallelisation have long been regarded as two different means of alleviating the prohibitive costs of parallel software development. Building on recent advances in both areas, Architecture-Independent Loop Parallelisation proposes a unified approach to the parallelisation of scientific computing code. This novel approach is based on the bulk-synchronous parallel model of computation, and succeeds in automatically generating parallel code that is architecture-independent, scalable, and of analytically predictable performance.

To make full use of the ever increasing hardware capabilities of modern com puters, it is necessary to speedily enhance the performance and reliability of the software as well, and often without having a suitable mathematical theory readily available. In the handling of more and more complex real-life numerical problems in all sorts of applications, a modern object-oriented de sign and implementation of software tools has become a crucial component. The considerable challenges posed by the demand for efficient object-oriented software in all areas of scientific computing make it necessary to exchange ideas and experiences from as many different sources as possible. Motivated by the success of the first meeting of this kind in Norway in 1996, we decided to organize another International Workshop on Modern Software Tools for Scientific Computing, often referred to as SciTools'98. This workshop took place in Oslo, Norway, September 14-16, 1998. The ob jective was again to provide an open forum for exchange and discussion of modern, state-of-the-art software techniques applied to challenging numerical problems. The organization was undertaken jointly by the research institute SINTEF Applied Mathematics, the Departments of Mathematics and Infor matics at the University of Oslo, and the company Numerical Objects AS.

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 Scientific Computation presents a methodology for designing parallel algorithms and writing parallel computer programs for modern computer architectures with multiple processors.

Parallel Scientific Computing and Optimization introduces new developments in the construction, analysis, and implementation of parallel computing algorithms. This book presents 23 self-contained chapters, including survey chapters and surveys, written by distinguished researchers in the field of parallel computing. Each chapter is devoted to some aspects of the subject: parallel algorithms for matrix computations, parallel optimization, management of parallel programming models and data, with the largest focus on parallel scientific computing in industrial applications. This volume is intended for scientists and graduate students specializing in computer science and applied mathematics who are engaged in parallel scientific computing.

Parallel Computing is a compelling vision of how computation can seamlessly scale from a single processor to virtually limitless computing power. Unfortunately, the scaling of application performance has not matched peak speed, and the programming burden for these machines remains heavy. This book represents the collected knowledge and experience of over 30 leading parallel computing researchers. They offer readers a complete sourcebook with solid coverage of parallel comuting hardware, programming considerations, algorithms, software and enabling technologies, as well as several parallel application case studies. (Midwest).

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.

In the last few years, courses on parallel computation have been developed and offered in many institutions in the UK, Europe and US as a recognition of the growing significance of this topic in mathematics and computer science. There is a clear need for texts that meet the needs of students and lecturers and this book, based on the author's lecture at ETH Zurich, is an ideal practical student guide to scientific computing on parallel computers working up from a hardware instruction level, to shared memory machines, and finally to distributed memory machines. Aimed at advanced undergraduate and graduate students in applied mathematics, computer science, and engineering, subjects covered include linear algebra, fast Fourier transform, and Monte-Carlo simulations, including examples in C and, in some cases, Fortran. This book is also ideal for practitioners and programmers.

The two volume set LNCS 7133 and LNCS 7134 constitutes the thoroughly refereed post-conference proceedings of the 10th International Conference on Applied Parallel and Scientific Computing, PARA 2010, held in Reykjavík, Iceland, in June 2010. These volumes contain three keynote lectures, 29 revised papers and 45 minisymposia presentations arranged on the following topics: cloud computing, HPC algorithms, HPC programming tools, HPC in meteorology, parallel numerical algorithms, parallel computing in physics, scientific computing tools, HPC software engineering, simulations of atomic scale systems, tools and environments for accelerator based computational biomedicine, GPU comput-

ing, high performance computing interval methods, real-time access and processing of large data sets, linear algebra algorithms and software for multicore and hybrid architectures in honor of Fred Gustavson on his 75th birthday, memory and multicore issues in scientific computing - theory and praxis, multicore algorithms and implementations for application problems, fast PDE solvers and a posteriori error estimates, and scalable tools for high performance computing.

In this text, students of applied mathematics, science and engineering are introduced to fundamental ways of thinking about the broad context of parallelism. The authors begin by giving the reader a deeper understanding of the issues through a general examination of timing, data dependencies, and communication. These ideas are implemented with respect to shared memory, parallel and vector processing, and distributed memory cluster computing. Threads, OpenMP, and MPI are covered, along with code examples in Fortran, C, and Java. The principles of parallel computation are applied throughout as the authors cover traditional topics in a first course in scientific computing. Building on the fundamentals of floating point representation and numerical error, a thorough treatment of numerical linear algebra and eigenvector/eigenvalue problems is provided. By studying how these algorithms parallelize, the reader is able to explore parallelism inherent in other computations, such as Monte Carlo methods.

Learn to solve scientific computing problems using Scala and its numerical computing, data processing, concurrency, and plotting libraries About This Book Parallelize your numerical computing code using convenient and safe techniques. Accomplish common high--performance, scientific computing goals in Scala. Learn about data visualization and how to create high-quality scientific plots in Scala Who This Book Is For Scientists and engineers who would like to use Scala for their scientific and numerical computing needs. A basic familiarity with undergraduate level mathematics and statistics is expected but not strictly required. A basic knowledge of Scala is required as well as the ability to write simple Scala programs. However, complicated programming concepts are not used in the book. Anyone who wants to explore using Scala for writing scientific or engineering software will benefit from the book. What You Will Learn Write and read a variety of popular file formats used to store scientific data Use Breeze for linear algebra, optimization, and digital signal processing Gain insight into Saddle for data analysis Use ScalaLab for interactive computing Quickly and conveniently write safe parallel applications using Scala's parallel collections Implement and deploy concurrent programs using the Akka framework Use the Wisp plotting library to produce scientific plots Visualize multivariate data using various visualization techniques In Detail Scala is a statically typed, Java Virtual Machine (JVM)-based language with strong support for functional programming. There exist libraries for Scala that cover a range of common scientific computing tasks – from linear algebra and numerical algorithms to convenient and safe parallelization to powerful plotting facilities. Learning to use these to perform common scientific tasks will allow you to write programs that are both fast and easy to write and main-

tain. We will start by discussing the advantages of using Scala over other scientific computing platforms. You will discover Scala packages that provide the functionality you have come to expect when writing scientific software. We will explore using Scala's Breeze library for linear algebra, optimization, and signal processing. We will then proceed to the Saddle library for data analysis. If you have experience in R or with Python's popular pandas library you will learn how to translate those skills to Saddle. If you are new to data analysis, you will learn basic concepts of Saddle as well. Well will explore the numerical computing environment called ScalaLab. It comes bundled with a lot of scientific software readily available. We will use it for interactive computing, data analysis, and visualization. In the following chapters, we will explore using Scala's powerful parallel collections for safe and convenient parallel programming. Topics such as the Akka concurrency framework will be covered. Finally, you will learn about multivariate data visualization and how to produce professional-looking plots in Scala easily. After reading the book, you should have more than enough information on how to start using Scala as your scientific computing platform Style and approach Examples are provided on how to use Scala to do basic numerical and scientific computing tasks. All the concepts are illustrated with more involved examples in each chapter. The goal of the book is to allow you to translate existing experience in scientific computing to Scala.

Topics in Parallel and Distributed Computing provides resources and guidance for those learning PDC as well as those teaching students new to the discipline. The pervasiveness of computing devices containing multicore CPUs and GPUs, including home and office PCs, laptops, and mobile devices, is making even common users dependent on parallel processing. Certainly, it is no longer sufficient for even basic programmers to acquire only the traditional sequential programming skills. The preceding trends point to the need for imparting a broad--based skill set in PDC technology. However, the rapid changes in computing hardware platforms and devices, languages, supporting programming environments, and research advances, poses a challenge both for newcomers and seasoned computer scientists. This edited collection has been developed over the past several years in conjunction with the IEEE technical committee on parallel processing (TCPP), which held several workshops and discussions on learning parallel computing and integrating parallel concepts into courses throughout computer science curricula. Contributed and developed by the leading minds in parallel computing research and instruction Provides resources and guidance for those learning PDC as well as those teaching students new to the discipline Succinctly addresses a range of parallel and distributed computing topics Pedagogically designed to ensure understanding by experienced engineers and newcomers Developed over the past several years in conjunction with the IEEE technical committee on parallel processing (TCPP), which held several workshops and discussions on learning parallel computing and integrating parallel concepts

Numerical algorithms, modern programming techniques, and parallel

computing are often taught serially across different courses and different textbooks. The need to integrate concepts and tools usually comes only in employment or in research - after the courses are concluded - forcing the student to synthesise what is perceived to be three independent subfields into one. This book provides a seamless approach to stimulate the student simultaneously through the eyes of multiple disciplines, leading to enhanced understanding of scientific computing as a whole. The book includes both basic as well as advanced topics and places equal emphasis on the discretization of partial differential equations and on solvers. Some of the advanced topics include wavelets, high-order methods, non-symmetric systems, and parallelization of sparse systems. The material covered is suited to students from engineering, computer science, physics and mathematics.

Automatic differentiation is a powerful technique for evaluating derivatives of functions given in the form of a high-level programming language such as Fortran, C, or C++. The program is treated as a potentially very long sequence of elementary statements to which the chain rule of differential calculus is applied over and over again. Combining automatic differentiation and the organizational structure of toolkits for parallel scientific computing provides a mechanism for evaluating derivatives by exploiting mathematical insight on a higher level. In these toolkits, algorithmic structures such as BLAS-like operations, linear and nonlinear solvers, or integrators for ordinary differential equations can be identified by their standardized interfaces and recognized as high-level mathematical objects rather than as a sequence of elementary statements. In this note, the differentiation of a linear solver with respect to some parameter vector is taken as an example. Mathematical insight is used to reformulate this problem into the solution of multiple linear systems that share the same coefficient matrix but differ in their right--hand sides. The experiments reported here use ADIC, a tool for the automatic differentiation of C programs, and PETSC, an object-oriented toolkit for the parallel solution of scientific problems modeled by partial differential equations.

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.

Parallel Computing for Da-

ta Science: With Examples in R, C++ and CUDA is one of the first parallel computing books to concentrate exclusively on parallel data structures, algorithms, software tools, and applications in data science. It includes examples not only from the classic "n observations, p variables" matrix format but also from time series,

Scientific computing has become an indispensable tool in numerous fields, such as physics, mechanics, biology, finance and industry. For example, it enables us, thanks to efficient algorithms adapted to current computers, to simulate, without the help of models or experimentations, the deflection of beams in bending, the sound level in a theater room or a fluid flowing around an aircraft wing. This book presents the scientific computing techniques applied to parallel computing for the numerical simulation of large-scale problems; these problems result from systems modeled by partial differential equations. Computing concepts will be tackled via examples. Implementation and programming techniques resulting from the finite element method will be presented for direct solvers, iterative solvers and domain decomposition methods, along with an introduction to MPI and OpenMP.

The book provides an introduction to common programming tools and methods in numerical mathematics and scientific computing. Unlike widely used standard approaches, it does not focus on any particular language but aims to explain the key underlying concepts. In general, new concepts are first introduced in the particularly user-friendly Python language and then transferred and expanded in various scientific programming environments from C / C ++, Julia and MATLAB to Maple. This includes different approaches to distributed computing. The fact that different languages are studied and compared also makes the book useful for mathematicians and practitioners trying to decide which programming language to use for which purposes.