Parallel Scientific Computing In C And Mpi A Seamless Approach To Parallel Algorithms And Their Implementation

Mathematics of Computing -- Parallelism.

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.

Parallel and High Performance Computing offers techniques guaranteed to boost your code's effectiveness. Summary Complex calculations, like training deep learning models or running large-scale simulations, can take an extremely long time. Efficient parallel programming can save hours—or even days—of computing time. Parallel and High Performance Computing shows you how to deliver faster run-times, greater scalability, and increased energy efficiency to your programs by mastering parallel techniques for multicore processor and GPU hardware. About the technology Write fast, powerful, energy efficient programs that scale to tackle huge volumes of data. Using parallel programming, your code spreads data processing tasks across multiple CPUs for radically better performance. With a little help, you can create software that maximizes both speed and efficiency. About the book Parallel and High Performance Computing offers techniques guaranteed to boost your code's effectiveness. You'll learn to evaluate hardware architectures and work with industry standard tools such as OpenMP and MPI. You'll master the data structures and algorithms best suited for high performance computing and learn techniques that save energy on handheld devices. You'll even run a massive tsunami simulation across a bank of GPUs. What's inside Planning a new parallel project Understanding differences in CPU and GPU architecture Addressing underperforming kernels and loops Managing applications with batch scheduling About the reader For experienced programmers proficient with a high-performance computing language like C, C++, or Fortran. About the author Robert Robey works at Los Alamos National Laboratory and has been active in the field of parallel computing for over 30 years. Yuliana Zamora is currently a PhD student and Siebel Scholar at the University of Chicago, and has lectured on programming modern hardware at numerous national conferences. Table of Contents PART 1 INTRODUCTION TO PARALLEL COMPUTING 1 Why parallel computing? 2 Planning for parallelization 3 Performance limits and profiling 4 Data design and performance models 5 Parallel algorithms and patterns PART 2 CPU: THE PARALLEL WORKHORSE 6 Vectorization: FLOPs for free 7 OpenMP that performs 8 MPI: The parallel backbone PART 3 GPUS: BUILT TO ACCELERATE 9 GPU architectures and concepts 10 GPU programming model 11 Directive-based GPU programming 12 GPU languages: Getting down to basics 13 GPU profiling and tools PART 4 HIGH PERFORMANCE COMPUTING ECOSYSTEMS 14 Affinity: Truce with the kernel 15 Batch schedulers: Bringing order to chaos 16 File operations for a parallel world 17 Tools and resources for better code

This is a 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.

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 projects. 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.

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 can be used by both IBM PC and Macintosh compatible computers. HTML files included on the CD-ROM 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 code use license is included.

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.

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 computing, 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.

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 Scientific Computing in C++ and MPIA Seamless Approach to Parallel Algorithms and Their ImplementationCambridge University Press

An Introduction to Parallel Programming, Second Edition presents a tried-and-true tutorial approach that shows students how to develop effective parallel programs with MPI, Pthreads and OpenMP. As the first undergraduate text to directly address compiling and running parallel programs on multi-core and cluster architecture, this second edition carries forward its clear explanations for designing, debugging and evaluating the performance of distributed and shared-memory programs while adding coverage of accelerators via new content on GPU programming and heterogeneous programming. New and improved user-friendly exercises teach students how to compile, run and modify example programs. Takes a tutorial approach, starting with small programming examples and building progressively to more challenging examples Explains how to develop parallel programs using MPI, Pthreads and OpenMP programming models A robust package of online ancillaries for instructors and students includes lecture slides, solutions manual, downloadable source code, and an image bank New to this edition: New chapters on GPU programming and heterogeneous programming New examples and exercises related to parallel algorithms

Software -- Programming Techniques.

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.

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.

This book differs from traditional numerical analysis texts in that it focuses on the motivation and ideas behind the algorithms presented rather than on detailed analyses of them. It presents a broad overview of methods and software for solving mathematical problems arising in computational modeling and data analysis, including proper problem formulation, selection of effective solution algorithms, and interpretation of results.? In the 20 years since its original publication, the modern, fundamental perspective of this book has aged well, and it continues to be used in the classroom. This Classics edition has been updated to include pointers to Python software and the Chebfun package, expansions on barycentric formulation for Lagrange polynomial interpretation and stochastic methods, and the availability of about 100 interactive educational modules that dynamically illustrate the concepts and algorithms in the book. Scientific Computing: An Introductory Survey, Second Edition is intended as both a textbook and a reference for computationally oriented disciplines that need to solve mathematical problems.

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.

Content Description #Includes bibliographical references and index.

Designed for undergraduates, An Introduction to High-Performance Scientific Computing assumes a basic knowledge of numerical computation and proficiency in Fortran or C programming and can be used in any science, computer science, applied mathematics, or engineering department or by practicing scientists and engineers, especially those associated with one of the national laboratories or

supercomputer centers. This text evolved from a new curriculum in scientific computing that was developed to teach undergraduate science and engineering majors how to use high-performance computing systems (supercomputers) in scientific and engineering applications. Designed for undergraduates, An Introduction to High-Performance Scientific Computing assumes a basic knowledge of numerical computation and proficiency in Fortran or C programming and can be used in any science, computer science, applied mathematics, or engineering department or by practicing scientists and engineers, especially those associated with one of the national laboratories or supercomputer centers. The authors begin with a survey of scientific computing and then provide a review of background (numerical analysis, IEEE arithmetic, Unix, Fortran) and tools (elements of MATLAB, IDL, AVS). Next, full coverage is given to scientific visualization and to the architectures (scientific workstations and vector and parallel supercomputers) and performance evaluation needed to solve large-scale problems. The concluding section on applications includes three problems (molecular dynamics, advection, and computerized tomography) that illustrate the challenge of solving problems on a variety of computer architectures as well as the suitability of a particular architecture to solving a particular problem. Finally, since this can only be a hands-on course with extensive programming and experimentation with a variety of architectures and programming paradigms, the authors have provided a laboratory manual and supporting software via anonymous ftp. Scientific and Engineering Computation series

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.

What does Google's management of billions of Web pages have in common with analysis of a genome with billions of nucleotides? Both apply methods that coordinate many processors to accomplish a single task. From mining genomes to the World Wide Web, from modeling financial markets to global weather patterns, parallel computing enables computations that would otherwise be impractical if not impossible with sequential approaches alone. Its fundamental role as an enabler of simulations and data analysis continues an advance in a wide range of application areas. Scientific Parallel Computing is the first textbook to integrate all the fundamentals of parallel computing in a single volume while also providing a basis for a deeper understanding of the subject. Designed for graduate and advanced undergraduate courses in the sciences and in engineering, computer science, and mathematics, it focuses on the three key areas of algorithms, architecture, languages, and their crucial synthesis in performance. The book's computational examples, whose math prerequisites are not beyond the level of advanced calculus, derive from a breadth of topics in scientific and engineering simulation and data analysis. The programming exercises presented early in the book are designed to bring students up to speed quickly, while the book later develops projects challenging enough to guide students toward research questions in the field. The new paradigm of cluster computing is fully addressed. A supporting web site provides access to all the codes and software mentioned in the book, and offers topical information on popular parallel computing systems. Integrates all the fundamentals of parallel computing essential for today's high-performance requirements Ideal for graduate and advanced undergraduate students in the sciences and in engineering, computer science, and mathematics Extensive programming and theoretical exercises enable students to write parallel codes quickly More challenging projects later in the book introduce research questions New paradigm of cluster computing fully addressed Supporting web site provides access to all the codes and software mentioned in the book

Ever-increasing size and complexity of software applications and libraries in parallel scientific computing is making implementation in the programming languages traditional for this field--FORTRAN 77 and C--impractical. The major impediment to the progression to a higher-level language such as C++ is attaining FORTRAN 77 or C performance, which is considered absolutely necessary by many practitioners. The use of template metaprogramming in C++, in the form of so-called expression templates to generate custom C++ code, holds great promise for getting C performance from C++ in the context of operations on array-like objects. Several sophisticated expression template implementations of parallel array-class libraries exist, and in certain circumstances their promise of performance is realized. Unfortunately this is not uniformly the case; this paper explores the major reasons that this is so.

The book serves as a first introduction to computer programming of scientific applications, using the high-level Python language. The exposition is example and problem-oriented, where the applications are taken from mathematics, numerical calculus, statistics, physics, biology and finance. The book teaches "Matlab-style" and procedural programming as well as object-oriented programming. High school mathematics is a required background and it is advantageous to study classical and numerical one-variable calculus in parallel with reading this book. Besides learning how to program computers, the reader will also learn how to solve mathematical problems, arising in various branches of science and engineering, with the aid of numerical methods and programming. By blending programming, mathematics and scientific applications, the book lays a solid foundation for practicing computational science. From the reviews: Langtangen ... does an excellent job of introducing programming as a set of skills in problem solving. He guides the reader into thinking properly about producing program logic and data structures for modeling real-world problems using objects and functions and embracing the object-oriented paradigm. ... Summing Up: Highly recommended. F. H. Wild III, Choice, Vol. 47 (8), April 2010 Those of us who have learned scientific programming in Python 'on the streets' could be a little jealous of students who have the opportunity to take a course out of Langtangen's Primer." John D. Cook, The Mathematical Association of America, September 2011 This book goes through Python in particular, and programming in general, via tasks that scientists will likely perform. It contains valuable information for students new to scientific computing and would be the perfect bridge between an introduction to programming and an advanced course on numerical methods or computational science. Alex Small, IEEE, CiSE Vol. 14 (2), March /April 2012 "This fourth edition is a wonderful, inclusive textbook that covers pretty much everything one needs to know to go from zero to fairly sophisticated scientific programming in Python..." Joan Horvath, Computing Reviews, March 2015

An overview of the most prominent contemporary parallel processing programming models, written in a unique tutorial style. With the coming of the parallel computing era, computer scientists have turned their attention to designing programming models that are suited for high-performance parallel computing and supercomputing systems. Programming parallel systems is complicated by the fact that multiple processing units are simultaneously computing and moving data. This book offers an overview of some of the most prominent parallel programming models used in high-performance computing and supercomputing systems today. The chapters describe the programming models in a unique tutorial style rather than using the formal approach taken in the research literature. The aim is to cover a wide range of parallel programming models, enabling the reader to understand what each has to offer. The book begins with a description of the Message Passing Interface (MPI), the most common parallel programming model for distributed memory computing. It goes on to cover one-sided communication models, ranging from low-level runtime libraries (GASNet, OpenSHMEM) to high-level programming models (UPC, GA, Chapel); task-oriented programming models (Charm++, ADLB, Scioto, Swift, CnC) that allow users to describe their computation and data units as tasks so that the runtime system can manage computation and data movement as necessary; and parallel programming models intended for on-node parallelism in the context of multicore architecture or attached accelerators (OpenMP, Cilk Plus, TBB, CUDA, OpenCL). The book will be a valuable resource for graduate students, researchers, and any scientist who works with data sets and large computations. Contributors Timothy Armstrong,

Michael G. Burke, Ralph Butler, Bradford L. Chamberlain, Sunita Chandrasekaran, Barbara Chapman, Jeff Daily, James Dinan, Deepak Eachempati, Ian T. Foster, William D. Gropp, Paul Hargrove, Wen-mei Hwu, Nikhil Jain, Laxmikant Kale, David Kirk, Kath Knobe, Ariram Krishnamoorthy, Jeffery A. Kuehn, Alexey Kukanov, Charles E. Leiserson, Jonathan Lifflander, Ewing Lusk, Tim Mattson, Bruce Palmer, Steven C. Pieper, Stephen W. Poole, Arch D. Robison, Frank Schlimbach, Rajeev Thakur, Abhinav Vishnu, Justin M. Wozniak, Michael Wilde, Kathy Yelick, Yili Zheng

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.

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.

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

Numerical Computation Using C is a four-chapter text guide for learning C language from the numerical analysis viewpoint. C is a general-purpose language that has been used in systems programming. The first chapter discusses the basic principles, logic, operators, functions, arrays, and structures of C language. The next two chapters deal with the uses of the so-called pointers in the C language, which is a variable that contains the address of some object in memory. These chapters also elaborate on several constructs to show how the use of C language can be fine-tuned. The last chapter highlights the practical aspects of C language. This book will be of value to computer scientists and mathematicians.

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 maintain. 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.

This highly acclaimed work, first published by Prentice Hall in 1989, is a comprehensive and theoretically sound treatment of parallel and distributed numerical methods. It focuses on algorithms that are naturally suited for massive parallelization, and it explores the fundamental convergence, rate of convergence, communication, and synchronization issues associated with such algorithms. This is an extensive book, which aside from its focus on parallel and distributed algorithms, contains a wealth of material on a broad variety of computation and optimization topics. It is an excellent supplement to several of our other books, including Convex Optimization Algorithms (Athena Scientific, 2015), Nonlinear Programming (Athena Scientific, 1999), Dynamic Programming and Optimal Control (Athena Scientific, 2012), Neuro-Dynamic Programming (Athena Scientific, 1996), and Network Optimization (Athena Scientific, 1998). The on-line edition of the book contains a 95-page solutions manual.

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.

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.

The era of practical parallel programming has arrived, marked by the popularity of the MPI and OpenMP software standards and the emergence of commodity clusters as the hardware platform of choice for an increasing number of organizations. This exciting new book,Parallel Programming in C with MPI and OpenMPaddresses the needs of students and professionals who want to learn how to design, analyze, implement, and benchmark parallel programs in C using MPI and/or OpenMP. It introduces a rock-solid design methodology with coverage of the most important MPI functions and OpenMP directives. It also demonstrates, through a wide range of examples, how to develop parallel programs that will execute efficiently on today's parallel platforms. If you are an instructor who has adopted the book and would like access to the additional resources, please contact your local sales rep. or Michelle Flomenhoft at: michelle_flomenhoft@mcgraw-hill.com.

Summary: This work combines selected papers from a July 2008 workshop held in Cetraro, Italy, with invited papers by international contributors. Material is in sections on algorithms and scheduling, architectures, GRID technologies, cloud technologies, information processing and applications, and HPC and GRID infrastructures for e-science. B&w maps, images, and screenshots are used to illustrate topics such as nondeterministic coordination using S-Net, cloud computing for on-demand grid resource provisioning, grid computing for financial applications, and the evolution of research and education

networks and their essential role in modern science. There is no subject index. The book's readership includes computer scientists, IT engineers, and managers interested in the future development of grids, clouds, and large-scale computing. Gentzsch is affiliated with the DEISA Project and Open Grid Forum, Germany.

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.

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.

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.

Parallel Computing for Data 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,

A clear illustration of how parallel computers can be successfully applied to large-scale scientific computations. This book demonstrates how a variety of applications in physics, biology, mathematics and other sciences were implemented on real parallel computers to produce new scientific results. It investigates issues of fine-grained parallelism relevant for future supercomputers with particular emphasis on hypercube architecture. The authors describe how they used an experimental approach to configure different massively parallel machines, design and implement basic system software, and develop algorithms for frequently used mathematical computations. They also devise performance models, measure the performance characteristics of several computers, and create a high-performance computing facility based exclusively on parallel computers. By addressing all issues involved in scientific problem solving, Parallel Computing Works! provides valuable insight into computational science for large-scale parallel architectures. For those in the sciences, the findings reveal the usefulness of an important experimental tool. Anyone in supercomputing and related computational fields will gain a new perspective on the potential contributions of parallelism. Includes over 30 full-color illustrations.

Looking back at the years that have passed since the realization of the very first electronic, multi-purpose computers, one observes a tremendous growth in hardware and software performance. Today, researchers and engi neers have access to computing power and software that can solve numerical problems which are not fully understood in terms of existing mathemati cal theory. Thus, computational sciences must in many respects be viewed as experimental disciplines. As a consequence, there is a demand for high quality, flexible software that allows, and even encourages, experimentation with alternative numerical strategies and mathematical models. Extensibil ity is then a key issue; the software must provide an efficient environment for incorporation of new methods and models that will be required in fu ture problem scenarios. The development of such kind of flexible software is a challenging and expensive task. One way to achieve these goals is to in vest much work in the design and implementation of generic software tools which can be used in a wide range of application fields. In order to provide a forum where researchers could present and discuss their contributions to the described development, an International Work shop on Modern Software Tools for Scientific Computing was arranged in Oslo, Norway, September 16-18, 1996. This workshop, informally referred to as Sci Tools '96, was a collaboration between SINTEF Applied Mathe matics and the Departments of Informatics and Mathematics at the Uni versity of Oslo.