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Scientific Computing

Gene H. Golub, James M. Ortega



Scientific Computing:

Numerical Methods in Scientific Computing Germund Dahlquist, Ake Björck, 2008-01-01 This new book from the authors of the classic book *Numerical Methods* addresses the increasingly important role of numerical methods in science and engineering. More cohesive and comprehensive than any other modern textbook in the field, it combines traditional and well-developed topics with other material that is rarely found in numerical analysis texts, such as interval arithmetic, elementary functions, operator series, convergence acceleration, and continued fractions. Although this volume is self-contained, more comprehensive treatments of matrix computations will be given in a forthcoming volume. A supplementary Website contains three appendices: an introduction to matrix computations, a description of Mulprec, a MATLAB multiple precision package, and a guide to literature, algorithms, and software in numerical analysis. Review questions, problems, and computer exercises are also included. For use in an introductory graduate course in numerical analysis and for researchers who use numerical methods in science and engineering.

Elements of Scientific Computing Aslak Tveito, Hans Petter Langtangen, Bjørn Frederik Nielsen, Xing Cai, 2010-09-24 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.

Guide to Scientific Computing Peter R. Turner, 2001 This book introduces the reader to many of the problems of scientific computing and the wide variety of methods used for their solutions. It discusses basic approaches and stimulates an appreciation of the need for numerical methods in solving different types of problems. For each of the problems presented, the author provides some mathematical justification and examples. These serve as practical evidence and motivation for the reader to follow. Practical justification of the methods is provided through computer examples and exercises. The book includes an introduction to MATLAB, but the code used is not intended to exemplify sophisticated or robust pieces of software; it is purely illustrative of the method under discussion.

Numerical Analysis in Modern Scientific Computing Peter Deuflhard, Andreas Hohmann, 2012-12-06 Mathematics is playing an ever more important role in the physical and biological sciences, provoking a blurring of boundaries between scientific disciplines and a resurgence of interest in the modern as well as the classical techniques of applied mathematics. This renewal of interest, both in research and teaching, has led to the establishment of the series *Texts in Applied Mathematics (TAM)*. The development of new courses is a natural consequence of a high level of excitement on the research frontier, as newer techniques, such as numerical and symbolic computer systems, dynamical systems, and chaos, mix with and reinforce the traditional methods of applied mathematics. Thus, the purpose of this

textbook series is to meet the current and future needs of these advances and to encourage the teaching of new courses TAM will publish textbooks suitable for use in advanced undergraduate and beginning graduate courses and will complement the Applied Mathematical Sciences AMS series which will focus on advanced textbooks and research level monographs

A Gentle Introduction to Scientific Computing Dan Stancescu, Long Lee, 2022-05-01 Scientific Computation has established itself as a stand alone area of knowledge at the borderline between computer science and applied mathematics Nonetheless its interdisciplinary character cannot be denied its methodologies are increasingly used in a wide variety of branches of science and engineering A Gentle Introduction to Scientific Computing intends to serve a very broad audience of college students across a variety of disciplines It aims to expose its readers to some of the basic tools and techniques used in computational science with a view to helping them understand what happens behind the scenes when simple tools such as solving equations plotting and interpolation are used To make the book as practical as possible the authors explore their subject both from a theoretical mathematical perspective and from an implementation driven programming perspective Features Middle ground approach between theory and implementation Suitable reading for a broad range of students in STEM disciplines Could be used as the primary text for a first course in scientific computing Introduces mathematics majors without any prior computer science exposure to numerical methods All mathematical knowledge needed beyond Calculus together with the most widely used Calculus notation and concepts is introduced in the text to make it self contained The erratum document for A Gentle Introduction to Scientific Computing can be accessed here

Scientific Computing Bertil Gustafsson, 2018-10-03 This book explores the most significant computational methods and the history of their development It begins with the earliest mathematical numerical achievements made by the Babylonians and the Greeks followed by the period beginning in the 16th century For several centuries the main scientific challenge concerned the mechanics of planetary dynamics and the book describes the basic numerical methods of that time In turn at the end of the Second World War scientific computing took a giant step forward with the advent of electronic computers which greatly accelerated the development of numerical methods As a result scientific computing became established as a third scientific method in addition to the two traditional branches theory and experimentation The book traces numerical methods journey back to their origins and to the people who invented them while also briefly examining the development of electronic computers over the years Featuring 163 references and more than 100 figures many of them portraits or photos of key historical figures the book provides a unique historical perspective on the general field of scientific computing making it a valuable resource for all students and professionals interested in the history of numerical analysis and computing and for a broader readership alike

Scientific Computing Michael T. Heath, 2018-11-14 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 *High-Performance Scientific Computing* Edoardo Di Napoli, Marc-André Hermanns, Hristo Iliev, Andreas Lintermann, Alexander Peyser, 2017-03-01 This book constitutes the thoroughly refereed post conference proceedings of the First JARA High Performance Computing Symposium JARA HPC 2016 held in Aachen Germany in October 2016 The 21 full papers presented were carefully reviewed and selected from 26 submissions They cover many diverse topics such as coupling methods and strategies in Computational Fluid Dynamics CFD performance portability and applications in HPC as well as provenance tracking for large scale simulations

Mastering Python Scientific Computing Hemant Kumar Mehta, 2015-09-23 A complete guide for Python programmers to master scientific computing using Python APIs and tools About This Book The basics of scientific computing to advanced concepts involving parallel and large scale computation are all covered Most of the Python APIs and tools used in scientific computing are discussed in detail The concepts are discussed with suitable example programs Who This Book Is For If you are a Python programmer and want to get your hands on scientific computing this book is for you The book expects you to have had exposure to various concepts of Python programming What You Will Learn Fundamentals and components of scientific computing Scientific computing data management Performing numerical computing using NumPy and SciPy Concepts and programming for symbolic computing using SymPy Using the plotting library matplotlib for data visualization Data analysis and visualization using Pandas matplotlib and IPython Performing parallel and high performance computing Real life case studies and best practices of scientific computing In Detail In today's world along with theoretical and experimental work scientific computing has become an important part of scientific disciplines Numerical calculations simulations and computer modeling in this day and age form the vast majority of both experimental and theoretical papers In the scientific method replication and reproducibility are two important contributing factors A complete and concrete scientific result should be reproducible and replicable Python is suitable for scientific computing A large community of users plenty of help and documentation a large collection of scientific libraries and environments great performance and good support makes Python a great choice for scientific computing At present Python is among the top choices for developing scientific workflow and the book targets existing Python developers to master this domain using Python The main things to learn in the book are the concept of scientific workflow managing scientific workflow data and performing computation on

this data using Python The book discusses NumPy SciPy SymPy matplotlib Pandas and IPython with several example programs Style and approach This book follows a hands on approach to explain the complex concepts related to scientific computing It details various APIs using appropriate examples *A First Course in Scientific Computing* Rubin Landau, Robyn Wangberg, 2005-05 Mathematica Fortran90 Maple and Java on the accompanying CD ROM in an interactive workbook format Scientific Computing with Python Claus Fuhrer, Jan Erik Solem, Olivier Verdier, 2021-07-30 Leverage this example packed comprehensive guide for all your Python computational needs Key Features Learn the first steps within Python to highly specialized concepts Explore examples and code snippets taken from typical programming situations within scientific computing Delve into essential computer science concepts like iterating object oriented programming testing and MPI presented in strong connection to applications within scientific computing Book Description Python has tremendous potential within the scientific computing domain This updated edition of Scientific Computing with Python features new chapters on graphical user interfaces efficient data processing and parallel computing to help you perform mathematical and scientific computing efficiently using Python This book will help you to explore new Python syntax features and create different models using scientific computing principles The book presents Python alongside mathematical applications and demonstrates how to apply Python concepts in computing with the help of examples involving Python 3.8 You'll use pandas for basic data analysis to understand the modern needs of scientific computing and cover data module improvements and built in features You'll also explore numerical computation modules such as NumPy and SciPy which enable fast access to highly efficient numerical algorithms By learning to use the plotting module Matplotlib you will be able to represent your computational results in talks and publications A special chapter is devoted to SymPy a tool for bridging symbolic and numerical computations By the end of this Python book you'll have gained a solid understanding of task automation and how to implement and test mathematical algorithms within the realm of scientific computing What you will learn Understand the building blocks of computational mathematics linear algebra and related Python objects Use Matplotlib to create high quality figures and graphics to draw and visualize results Apply object oriented programming OOP to scientific computing in Python Discover how to use pandas to enter the world of data processing Handle exceptions for writing reliable and usable code Cover manual and automatic aspects of testing for scientific programming Get to grips with parallel computing to increase computation speed Who this book is for This book is for students with a mathematical background university teachers designing modern courses in programming data scientists researchers developers and anyone who wants to perform scientific computation in Python Introduction to High Performance Scientific Computing David L. Chopp, 2019-03-01 Based on a course developed by the author Introduction to High Performance Scientific Computing introduces methods for adding parallelism to numerical methods for solving differential equations It contains exercises and programming projects that facilitate learning as well as examples and discussions based on the C programming language with additional comments

for those already familiar with C The text provides an overview of concepts and algorithmic techniques for modern scientific computing and is divided into six self contained parts that can be assembled in any order to create an introductory course using available computer hardware Part I introduces the C programming language for those not already familiar with programming in a compiled language Part II describes parallelism on shared memory architectures using OpenMP Part III details parallelism on computer clusters using MPI for coordinating a computation Part IV demonstrates the use of graphical programming units GPUs to solve problems using the CUDA language for NVIDIA graphics cards Part V addresses programming on GPUs for non NVIDIA graphics cards using the OpenCL framework Finally Part VI contains a brief discussion of numerical methods and applications giving the reader an opportunity to test the methods on typical computing problems

Scientific Computing Gene H. Golub, James M. Ortega, 2014-06-28 This book introduces the basic concepts of parallel and vector computing in the context of an introduction to numerical methods It contains chapters on parallel and vector matrix multiplication and solution of linear systems by direct and iterative methods It is suitable for advanced undergraduate and beginning graduate courses in computer science applied mathematics and engineering Ideally students will have access to a parallel or Vector computer but the material can be studied profitably in any case Gives a modern overview of scientific computing including parallel and vector computation Introduces numerical methods for both ordinary and partial differential equations Has considerable discussion of both direct and iterative methods for linear systems of equations including parallel and vector algorithms Covers most of the main topics for a first course in numerical methods and can serve as a text for this course

A First Course in Scientific Computing Rubin Landau, 2011 This book offers a new approach to introductory scientific computing It aims to make students comfortable using computers to do science to provide them with the computational tools and knowledge they need throughout their college careers and into their professional careers and to show how all the pieces can work together Rubin Landau introduces the requisite mathematics and computer science in the course of realistic problems from energy use to the building of skyscrapers to projectile motion with drag He is attentive to how each discipline uses its own language to describe the same concepts and how computations are concrete instances of the abstract Landau covers the basics of computation numerical analysis and programming from a computational science perspective The first part of the printed book uses the problem solving environment Maple as its context with the same material covered on the accompanying CD as both Maple and Mathematica programs the second part uses the compiled language Java with equivalent materials in Fortran90 on the CD and the final part presents an introduction to LaTeX replete with sample files Providing the essentials of computing with practical examples A First Course in Scientific Computing adheres to the principle that science and engineering students learn computation best while sitting in front of a computer book in hand in trial and error mode Not only is it an invaluable learning text and an essential reference for students of mathematics engineering physics and other sciences but it is also a consummate model for future textbooks in

computational science and engineering courses A broad spectrum of computing tools and examples that can be used throughout an academic career Practical computing aimed at solving realistic problems Both symbolic and numerical computations A multidisciplinary approach science math computer science Maple and Java in the book itself Mathematica Fortran90 Maple and Java on the accompanying CD in an interactive workbook format *Numerical Recipes 3rd Edition* William H. Press, 2007-09-06 Do you want easy access to the latest methods in scientific computing This greatly expanded third edition of Numerical Recipes has it with wider coverage than ever before many new expanded and updated sections and two completely new chapters The executable C code now printed in colour for easy reading adopts an object oriented style particularly suited to scientific applications Co authored by four leading scientists from academia and industry Numerical Recipes starts with basic mathematics and computer science and proceeds to complete working routines The whole book is presented in the informal easy to read style that made earlier editions so popular Highlights of the new material include a new chapter on classification and inference Gaussian mixture models HMMs hierarchical clustering and SVMs a new chapter on computational geometry covering KD trees quad and octrees Delaunay triangulation and algorithms for lines polygons triangles and spheres interior point methods for linear programming MCMC an expanded treatment of ODEs with completely new routines and many new statistical distributions For support or to subscribe to an online version please visit www.nr.com

An Introduction to Scientific Computing Ionut Danaila, Pascal Joly, Sidi Mahmoud Kaber, Marie Postel, 2007-12-03 This book demonstrates scientific computing by presenting twelve computational projects in several disciplines including Fluid Mechanics Thermal Science Computer Aided Design Signal Processing and more Each follows typical steps of scientific computing from physical and mathematical description to numerical formulation and programming and critical discussion of results The text teaches practical methods not usually available in basic textbooks numerical checking of accuracy choice of boundary conditions effective solving of linear systems comparison to exact solutions and more The final section of each project contains the solutions to proposed exercises and guides the reader in using the MATLAB scripts available online

An Introduction to High-performance Scientific Computing, 1996 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 **Scientific Computing and Differential Equations** Gene H. Golub,James M. Ortega,2014-06-28 Scientific Computing and Differential Equations An Introduction to Numerical Methods is an excellent complement to Introduction to Numerical Methods by Ortega and Poole The book emphasizes the importance of solving differential equations on a computer which comprises a large part of what has come to be called scientific computing It reviews modern scientific computing outlines its applications and places the subject in a larger context This book is appropriate for upper undergraduate courses in mathematics electrical engineering and computer science it is also well suited to serve as a textbook for numerical differential equations courses at the graduate level An introductory chapter gives an overview of scientific computing indicating its important role in solving differential equations and placing the subject in the larger environment Contains an introduction to numerical methods for both ordinary and partial differential equations Concentrates on ordinary differential equations especially boundary value problems Contains most of the main topics for a first course in numerical methods and can serve as a text for this course Uses material for junior senior level undergraduate courses in math and computer science plus material for numerical differential equations courses for engineering science students at the graduate level **Parallel Processing for Scientific Computing** Michael A. Heroux,Padma Raghavan,Horst D. Simon,2006-01-01 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

Large Scale Scientific Computing Deuffhard, 2012-12-06 In this book the new and rapidly expanding field of scientific computing is understood in a double sense as computing for scientific and engineering problems and as the science of doing such computations Thus scientific computing touches at one side mathematical modelling in the various fields of applications and at the other side computer science As soon as the mathematical models describe the features of real life processes in sufficient detail the associated computations tend to be large scale As a consequence interest more and more focusses on such numerical methods that can be expected to cope with large scale computational problems Moreover given the algorithms which are known to be efficient on a traditional computer the question of implementation on modern supercomputers may get crucial The present book is the proceedings of a meeting on Large Scale Scientific Computing that was held at the Oberwolfach Mathematical Institute July 14-19 1985 under the auspices of the Sonderforschungsbereich 123 of the University of Heidelberg Participants included applied scientists with computational interests numerical analysts and experts on modern parallel computers The purpose of the meeting was to establish a common understanding of recent issues in scientific computing especially in view of large scale problems Fields of applications which have been covered included semiconductor design chemical combustion flow through porous media climatology seismology fluid dynamics tomography rheology hydro power plant optimization subwily control space technology

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