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

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JONAH STEVENS

Guide to Scientific Computing in C++
Lulu.com
Written by high performance computing (HPC) experts, Introduction to High Performance Computing for Scientists and Engineers provides a solid introduction to current mainstream computer architecture, dominant parallel programming models, and useful optimization strategies for scientific HPC. From working in a scientific computing center, the authors gained a unique perspective on the requirements and attitudes of users as well as manufacturers of parallel computers. The text first introduces the architecture of modern cache-based microprocessors and discusses their inherent performance limitations, before describing general optimization strategies for serial code on cache-based architectures. It next covers shared- and distributed-memory parallel computer architectures and the

most relevant network topologies. After discussing parallel computing on a theoretical level, the authors show how to avoid or ameliorate typical performance problems connected with OpenMP. They then present cache-coherent non-uniform memory access (ccNUMA) optimization techniques, examine distributed-memory parallel programming with message passing interface (MPI), and explain how to write efficient MPI code. The final chapter focuses on hybrid programming with MPI and OpenMP. Users of high performance computers often have no idea what factors limit time to solution and whether it makes sense to think about optimization at all. This book facilitates an intuitive understanding of performance limitations without relying on heavy computer science knowledge. It also prepares readers for studying more advanced literature. Read about the authors' recent honor: Informatics Europe Curriculum Best Practices Award for Parallelism and Concurrency.

Introduction to High Performance Scientific Computing Springer Science & Business Media

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.

An Introduction to High-performance Scientific Computing Springer Science & Business Media

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. *Introduction to High Performance Computing for Scientists and Engineers* CRC 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.

An Introduction to Parallel and Vector Scientific Computation CRC Press

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

Parallel Scientific Computation CRC Press

This book constitutes the refereed proceedings of the 7th International Conference on Applied Parallel Computing, PARA 2004, held in June 2004. The 118 revised full papers presented together with five invited lectures and 15 contributed talks were carefully reviewed and selected for inclusion in the proceedings. The papers are organized in topical sections.

Handbook of Parallel Computing SIAM

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.

Introduction to Parallel Programming OUP Oxford

This book concerns programming techniques like object-oriented programming and generic (template) programming. These modern techniques have proven to increase flexibility, modularization, code reuse and improve maintenance of large numerical codes. The book contains 11 refereed and comprehensive chapters on major subjects in computational science and engineering: quality measurement of numerical software, high-performance numerical computations with C++ without sacrificing efficiency, a balanced discussion of Java in scientific computing, object-oriented design of direct sparse solvers, geometric kernels in geographical information systems, and tools for error estimation in finite element methods, tools for validating computational results, and how to simplify the implementation of highly complex mathematical model for material processing.

Numerical Solution of Partial Differential Equations on Parallel Computers Morgan Kaufmann
Since the dawn of computing, the quest for a better understanding of Nature has been a driving force for technological development. Groundbreaking achievements by great scientists have paved the way from the abacus to the supercomputing power of today. When trying to replicate Nature in the computer's silicon test tube, there is need for precise and computable process descriptions. The scienti?c ?elds of Ma- ematics and Physics provide a powerful vehicle for such descriptions in terms of Partial Differential Equations (PDEs). Formulated as such equations, physical laws can become subject to computational and analytical studies. In the computational setting, the equations can be discreti ed for ef?cient solution on a computer, leading to valuable tools for simulation of natural and man-made processes. Numerical so- tion of PDE-based mathematical models has been an important research topic over centuries, and will remain so for centuries to come. In the context of computer-based simulations, the quality of the computed results is directly connected to the model's complexity and the number of data points used for the computations.

Therefore, computational scientists tend to ?ll even the largest and most powerful computers they can get access to, either by increasing the si e of the data sets, or by introducing new model terms that make the simulations more realistic, or a combination of both. Today, many important simulation problems can not be solved by one single computer, but calls for parallel computing.

Modern Software Tools for Scientific Computing Springer Science & Business Media

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.

Computing in Object-Oriented Parallel Environments CRC Press

This is a textbook that teaches the bridging topics between numerical analysis, parallel computing, code performance, large scale applications.

Scientific Computing Springer

The book provides an introduction to common programming tools and methods in numerical mathematics and scientific computing. Unlike standard approaches, it does not focus on any specific language, but aims to explain the underlying ideas. Typically, new concepts are first introduced in the particularly user-friendly Python language and then transferred and extended in various programming

environments from C/C++, Julia and MATLAB to Maple and Mathematica. This includes various approaches to distributed computing. By examining and comparing different languages, the book is also helpful for mathematicians and practitioners in deciding which programming language to use for which purposes. At a more advanced level, special tools for the automated solution of partial differential equations using the finite element method are discussed. On a more experimental level, the basic methods of scientific machine learning in artificial neural networks are explained and illustrated.

Applied Parallel Computing MIT Press

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.
Introduction to High Performance Scientific Computing Cambridge University Press
The ability of parallel computing to process large data sets and handle time-consuming operations has resulted in unprecedented advances in biological and scientific computing, modeling, and simulations. Exploring these recent developments, the Handbook of Parallel Computing: Models, Algorithms, and Applications provides comprehensive coverage on a
Introduction to the Tools of Scientific Computing Springer Nature
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.

Elements of Scientific Computing Springer

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

Topics in Parallel and Distributed Computing

Oxford University Press

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.

Introduction to Parallel Computing MIT Press 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.

Applied Parallel Computing Cambridge University Press 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.

An Introduction to Parallel Programming Packt Publishing Ltd

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