Advanced Computational Infrastructures for Parallel and Distributed Adaptive Applications
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Edited by
Manish Parashar
Xiaolin Li
To our parents....
Shyam and Shashi – Manish Parashar
Guangdong and Meixian – Xiaolin Li
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Preface

INTRODUCTION

The last decade has witnessed a dramatic increase in computing, networking, and storage technologies. In the meantime, the emerging large-scale adaptive scientific and engineering applications are requiring an increasing amount of computing and storage resources to provide new insights into complex systems. Furthermore, dynamically adaptive techniques are being widely used to address the intrinsic heterogeneity and high dynamism of the phenomena modeled by these applications. Adaptive techniques have been applied to real-world applications in a variety of scientific and engineering disciplines, including computational fluid dynamics, subsurface and oil-reservoir simulations, astronomy, relativity, and weather modeling. The increasing complexity, dynamism, and heterogeneity of these applications coupled with similarly complex and heterogeneous parallel and distributed computing systems have led to the development and deployment of advanced computational infrastructures that provide programming, execution, and runtime management support for such large-scale adaptive implementations. The objective of this book is to investigate the state of the art in the design, architectures, and implementations of such advanced computational infrastructures and the applications they support.

This book presents the state of the art in advanced computational infrastructures for parallel and distributed adaptive applications and provides insights into recent research efforts and projects. The objective of this book is to provide a comprehensive discussion of the requirements, design challenges, underlying design philosophies, architectures, and implementation and deployment details of the advanced computational infrastructures. It presents a comprehensive study of the design, architecture, and implementation of advanced computational infrastructures as well as the adaptive applications developed and deployed using these infrastructures from different perspectives, including system architects, software engineers, computational scientists, and application scientists. Furthermore, the book includes descriptions and experiences pertaining to the realistic modeling of adaptive applications on parallel and distributed systems. By combining a “bird’s eye view” with the “nitty-gritty” of advanced computational infrastructures, this book will serve as a comprehensive cross-disciplinary reference and a unique and valuable resource for students, researchers, and professionals alike.
We believe that this book can be used as a textbook for advanced courses in computational science and software/systems engineering for senior undergraduate and graduate students. It can also serve as a valuable reference for computational scientists, computer scientists, industry professionals, software developers, and other researchers in the areas of computational science, numerical methods, computer science, high-performance computing, parallel/distributed computing, and software engineering.

OVERVIEW OF THE BOOK

The book is organized in three separate parts. Part I titled “Adaptive Applications in Science and Engineering” focuses on high-performance adaptive scientific applications and includes chapters that describe high-impact, real-world application scenarios. The goal of this part of the book is to emphasize the need for advanced computational engines as well as outline their requirements. Part II titled “Adaptive Computational Infrastructures” includes chapters describing popular and widely used adaptive computational infrastructures. Part III is titled “Dynamic Partitioning and Adaptive Runtime Management Frameworks” focuses on the more specific partitioning and runtime management schemes underlying these computational toolkits. The three parts are described in more detail below.

Part I consists of seven chapters. Chapter 2 presents the use of adaptive mesh refinement techniques in large-scale fusion simulations modeled using magnetohydrodynamics (MHD). The emphasis of this work is on understanding the large-scale macroscopic processes involved in the redistribution of mass inside a tokamak during pellet injection and to support experimentation using ITER. Chapter 3 introduces adaptive models and parallel computing engines for subsurface imaging such as hydraulic tomography. Chapter 4 proposes a new parallel imaging algorithm and its implementation in oil reservoir simulations. The algorithm is based on decomposing the observed seismic data into plane wave components that correlate to angles of incidence in the subsurface and the degree of lateral variability. Chapter 5 focuses on assessments of uncertainty in climate models and climate prediction. Chapter 6 focuses on high-fidelity computational fluid dynamics (CFD) models for hazardous airborne materials in urban environments. The rapid embedded boundary gridding method in AMR is proposed to support efficient adaptive operations for this application. Chapter 7 presents the parallel adaptive simulation of cardiac fluid dynamics using the immersed boundary method and an unstructured adaptive mesh refinement technique. Chapter 8 introduces quantum chromodynamics and presents a scalable implementation on the IBM BlueGene/L supercomputer. The work presented in this chapter was awarded the 2006 Gordon Bell Special Achievement Award.

Part II consists of six chapters. Chapter 9 presents the SCIJump problem solving environment (PSE), which builds on its successful predecessor SCIRun and is based on the DOE common component architecture (CCA) scientific component model.
SCIJump supports multiple component models under a metacomponent model. Chapter 10 describes the Uintah computational framework, which provides a set of parallel software components and libraries that facilitate the solution of partial differential equations (PDEs) on structured AMR (SAMR) grids. This framework uses an explicit representation of parallel computation and communication to enable integration of parallelism across multiple simulation methods. Chapter 11 focuses on the complexity of parallel adaptive finite element applications and describes the Sierra Framework, which supports a diverse set of finite element and finite volume engineering analysis codes. Chapter 12 presents the grid adaptive computational engine (GrACE), an object-oriented framework supporting the large-scale SAMR application, and providing support dynamic partitioning, scheduling, and automatic data migration. Over the years, GrACE has evolved into a widely used tool for supporting autonomic partitioning and runtime management of large-scale adaptive applications. Chapter 13 introduces the adaptive MPI model and presents an implementation using the Charm++ framework. An intelligent adaptive runtime system using migratable objects and various adaptive strategies is presented in this chapter. Chapter 14 presents the Seine framework for data/code coupling for large-scale coupled parallel scientific simulations. Seine provides the high-level abstraction as well as efficient runtime mechanisms to support MXN data redistributions required by such coupled applications.

Part III consists of eight chapters. Chapter 15 presents a hypergraph approach for dynamic partitioning and load balancing in scientific applications. Chapter 16 presents the PART framework and its mesh partitioning algorithms that can support scientific applications across geographically distributed systems. Chapter 17 presents a meshing partitioning framework, called variable partition inertia (VPI), for repartitioning adaptive unstructured meshes considering resource and application heterogeneity. Chapter 18 presents the Nature + Fable framework, a hybrid and flexible partitioning tool dedicated to structured grid hierarchies. Nature + Fable is shown to effectively cope with demanding, complex, and realistic SAMR applications. Chapter 19 proposes and implements a flexible mesh database based on a hierarchical domain decomposition to partition and manage evolving adaptive unstructured meshes. Chapter 20 presents a hybrid runtime management framework (HRMS) that provides a suite of partitioning and managing strategies. HRMS decomposes computational domain and selects an appropriate partitioner for each partition based on the partition’s local characteristics and requirements. Chapter 21 presents an autonomic programming framework PARM, which can dynamically self-configure the application execution environment to exploit the heterogeneity and the dynamism of the application execution states. Chapter 22 presents the DistDLB framework, which is equipped with hierarchical load balancing algorithms to support global balancing and local balancing phases. DistDLB is specifically targeted to SAMR simulations in cosmology.

Once again, the objective of this book is to investigate the state of the art in the design, architectures, and implementations of such advanced computational infrastructures and the applications they support. We do hope that it will lead to new insights into the underlying concepts and issues, current approaches and research
efforts, and outstanding challenges of the field and will inspire further research in this promising area.

ACKNOWLEDGMENTS

This book has been made possible due to the efforts and contributions of many individuals. First and foremost, we would like to acknowledge all the contributors for their tremendous efforts in putting together excellent chapters that are comprehensive, informative, and timely. We would like to thank the reviewers for their excellent comments and suggestions. We would also like to thank Professor Albert Zomaya for the opportunity to edit this book as part of the Wiley Book Series on Parallel and Distributed Computing and to Michael Christian and the rest of the team at John Wiley & Sons, Inc. for patiently helping us put this book together. Finally, we would like to acknowledge the support of our families and would like to dedicate this book to them.

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Manish has coauthored over 250 technical papers in international journals and conferences, has coauthored/edited over 20 books and proceedings, and has contributed to several others, all in the broad area of computational science and applied parallel and distributed computing.

Manish received a BE degree in Electronics and Telecommunications from Bombay University, India, and MS and PhD degrees in Computer Engineering from Syracuse University. For more information, please visit http://www.ece.rutgers.edu/~parashar/.
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