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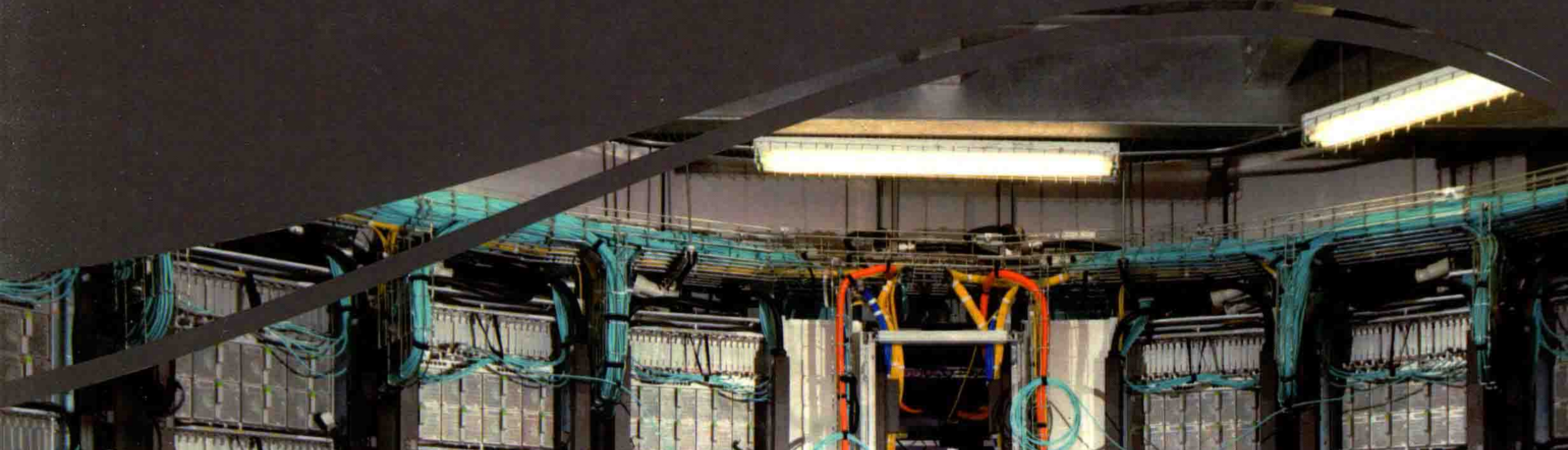
Research and Applications in Global Supercomputing



Richard S. Segall, Jeffrey S. Cook, and Qingyu Zhang

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Research and Applications in Global Supercomputing

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Preface

Supercomputers are the fastest computers and the backbone of Computational Sciences. By processing and generating vast amounts of data with unparalleled speed, they make new developments and research possible. The hardware structure or the architecture of supercomputers determines to a large extent the efficiency of supercomputing systems. Another important element that is considered is the ability of the compilers to generate efficient code to be executed on a given hardware platform.

While the supercomputers of the 1970s used only a few processors and the supercomputers by the end of the 20th century were massively parallel computing systems composed of tens of thousands of processors, the supercomputers of the 21st century can use over 100,000 processors connected by fast connections.

This book is designed to cover a broad range of topics in the field of supercomputing. As a result, it will be an excellent source on this topic. It is primarily intended for professionals, researchers, students, and practitioners who want to more fully understand the realm and technology of supercomputing and how it has been used to solve large-scale research problems in a multitude of disciplines. Because each chapter is designed to be stand-alone, the reader can focus on the topics that most interest him/her.

Supercomputers are used today for highly intensive calculation tasks for projects ranging from quantum physics, weather forecasting, molecular modeling, and physical simulations. Supercomputers can be used for simulations of airplanes in wind tunnels, detonations of nuclear weapons, splitting electrons, and helping researchers study how drugs combat the swine flu virus. Supercomputing can be in the form of grid computing, in which the processing power of a large number of computers is distributed, or in the form of computer clusters, in which a large number of processors are used in close proximity to each other.

In 2012, the Cray XK7 "Titan" at the United States Department of Energy (DOE) at Oak Ridge National Laboratory (ORNL) located in Tennessee was the fastest supercomputer in the world at 17.59 petaflops, consuming 8209 kilowatts of power using 560,640 cores (Top500, 2012). However, in 2014, according to the Top500 listing of November 2013, China outplaced the United States with the fastest supercomputer named Tianhe-2 for the "MilkyWay-2" built by NUDT and located at National Super Computer Center in Guangzhou with 33.86 petaflops consuming 17,808 kilowatts of power with 3,120,000 cores (Top500, 2013; see Appendix).

According to Wikipedia webpages titled "Supercomputing in India," the Indian Government has proposed to commit 2.5 billion in Unites States Dollars (USD) to supercomputing research during the 12th five-year plan period (2012-2017). The project will be handled by Indian Institute of Science (IISc), Bangalore. Additionally, it was later revealed that India plans to develop a supercomputer with processing power in the exaflop range (Supercomputing in India, n.d.).

The objective of this book is to present the concepts of supercomputing, explore its technologies and their applications, and develop a broad understanding of issues pertaining to the use of supercomputing in multidisciplinary fields. The book aims to highlight the historical and technical background; architecture; programming systems; storage, visualization, analytics, state of practice in industry, universities, and government; and numerous applications ranging from such areas as computational earth and atmospheric sciences to computational medicine.

Readers would utilize this book as a unified presentation of a spectrum of up-to-date research and applications topics on supercomputing. The collection of chapters could interest the readers to do subsequent research in supercomputing, as well as be used in teaching courses in supercomputing.

The book is focused on the structure, practice, and applications of supercomputing such as represented by the following topics: background of supercomputing; supercomputing architecture; clouds, clusters, and grids; programming systems for supercomputers; storage, visualization, and analytics for supercomputers including data mining for high performance computing; state of practice of supercomputers; and applications of supercomputers from bioinformatics to data-enabled social science.

A special novel feature of this book is that it contains an elaborate and descriptive Appendix of the "Top 500 Supercomputers in the World" and their rankings at the time of the publication of this book.

Section 1 consists of three chapters on "Overview to Global Supercomputing and its Current Challenges."

Chapter 1, "Overview of Global Supercomputing," by Richard S. Segall and Neha Gupta, provides an overview of global supercomputing and also as an introduction to the entire book of edited chapters. The subsequent chapters of this book include further discussion of Seymore Cray, the father of supercomputing, and the history of supercomputing from past to present to year 2050, and a history of supercomputing and supercomputer centers. The subsequent chapters include detailed studies of applications of supercomputing to nuclear power, nano-materials, steganography, cloud computing, leadership, sequence analysis and genome annotation, population genetics, programming paradigms, modeling of biological systems, renewable energy network design and optimization, data mining, philosophical logic perspective, a philosophy of their language, and current challenges across multiple domains of computational science. The reader is referred to the Appendix of this book for more information about each of the top 500 supercomputers in the world.

Chapter 2, "History of Supercomputing and Supercomputer Centers," by Jeffrey Cook and Neha Gupta, discusses various aspects of supercomputing, including the need for supercomputing and the challenges associated with supercomputing in terms of the cost and time. The chapter also presents the evolution of Seymour Cray's research beginning with the discovery of CDC 1604, CDC 6600, and CDC 7600 in 1960s to Star 100 in 1974, Cray 1 in 1976, CMOS ETA-10 in 1987, ILLIAC IV in 1976, Cray X-MP in 1982, Cray 2 in 1985, Cray Y-MP in 1988, Cray 3, and then the Cray era during the time period of years 2000 until today. Later, a discussion of the contributions of companies like Fujitsu, Hitachi, Intel, and NEC in supercomputing are provided.

Supercomputing and its dominance in healthcare are displayed by a brief discussion of a section on this topic. History of Supercomputing Center at Florida State University, Minnesota Supercomputing Center, and Moscow University Supercomputing Center are discussed among various equally important supercomputing centers globally. Dell's contributions in the evolution of supercomputing is also discussed in this chapter. A section on Petaflop supercomputing in 21st century and current exascale computing challenges are described coherently. The chapter highlights in a positive direction the current global supercomputing centers in the Top 500 list, the current trends in supercomputing, and the bright future of supercomputing.

Chapter 3 is titled "Applications and Current Challenges of Supercomputing across Multiple Domains of Computational Sciences," by Neha Gupta. Supercomputing has been of utmost importance since it was discovered because it has enabled crucial advances in national defense and safety, scientific discovery, manufacturing, etc. The current challenges of supercomputers across most of the computational sciences domains are discussed here that would enable a positive future direction. It is therefore obvious that the supercomputers are super smart digital computers having various achievements both in the past and in the bright future. For instance, a simple Google search is built on the usage of MapReduce™ paradigm that is a useful application of supercomputing. However, despite consistent increases in the capability, supercomputing systems are still inadequate to meet the computational needs of various projects.

The challenges discussed in this chapter are achievable by devising new architectures of supercomputers, something that is much faster, portable, and adaptable to most of the projects of all the subjects. Hence, it becomes imperative that novel research is applied that can produce more and more powerful supercomputing systems. The current status of supercomputing and limitations that forms the basis for future work are discussed in this chapter for computational areas ranging from bioinformatics and computational biology to computational design optimization for manufacturing. The future ideas which can be applied efficiently with the availability of good computing resources are explained coherently in this chapter.

Section 2 consists of seven chapters on "Supercomputing Applications."

Chapter 4, "Accelerated Discovery and Design of Nano-Material Applications in Nuclear Power by Using High Performance Scientific Computing," by Liviu Popa-Simil, presents a summary of nanomaterials, nano-technologies, and associated physics and engineering capable of improving nuclear power performance, motivation to use high performance scientific computing, and examples of different nuclear energy-related problems and their solutions that led to accelerated development of high-performance scientific computing.

Chapter 5, "Using High Performance Scientific Computing to Accelerate the Discovery and Design of Nuclear Power Applications," by Liviu Popa-Simil, discusses available architectures and solution approaches, presentation of the common sense, and practicality of developing the supercomputer architectures, issues in current supercomputing landscape, modern trends in high performance scientific computing with respect to nuclear power applications, and examples of future extreme-scale, multi-process, multiphenomena high performance supercomputing. This chapter indicates that the future belongs to quantum computers, with far greater capabilities, if we succeed to understand some fundamental problems that are now hot research subjects. The author of this chapter feels that the term Central Processing Unit (CPU) might be replaced by a Quantum Processing Unit, and the terms memory and communication interface might be replaced by their quantum equivalents, respectively.

Chapter 6, "Applications of Supercomputers in Sequence Analysis and Genome Annotation," by Gerard G. Dumancas, discusses that sequence alignment and genome annotation are among the most commonly used techniques in the area of genetics and bioinformatics. With the emergence of a large sequence of genomic data, scientists are confronted with computational burden in these two fields. Supercomputers facilitate in the ease of analyses in these two areas by reducing computational time. Synchronizing the threads in supercomputing processes and the use of massively parallel, distributed memory supercomputers enable researchers to do comparative genomics on large datasets, eventually reducing computational time.

Chapter 7, "Applications of Supercomputers in Population Genetics," by Gerard G. Dumancas, discusses how supercomputers play a critical role in the success of the field of population genetics. This field is the study of the frequency and interaction of alleles and genes in populations and how this allele frequency distribution changes over time as a result of evolutionary processes such as natural selection, genetic drift, and mutation. This field has become essential in the foundation of modern evolutionary synthesis. Traditionally regarded as a highly mathematical discipline, its modern approach comprises more than the theoretical, lab, and fieldwork.

Chapter 8, "Supercomputers in Modeling of Biological Systems," by Randall Maples, Sindhura Ramasahayam, and Gerard G. Dumancas, discusses computational methods for protein structure prediction, including that of homology modeling, and fold recognition or threading, and computational methods for protein-ligand binding site identification, including that of protein-surface interactions. This chapter discusses that protein modeling is playing a more and more important role in protein and peptide sequences due to improvements in modeling methods, advances in computer technology, and the huge amount of biological data becoming available. These modeling tools can pave the way to future research directions in predicting the structure, functions, and mechanisms of novel proteins.

This chapter discusses that although there has been progress in using supercomputers for the prediction of biological systems (i.e. proteins), there have been challenges facing the scientists today, which include refining comparative models so that these could match experimental accuracy, search for more algorithms that can predict the structure of very large proteins, calculations of absolute binding free energies in protein-ligand binding, as well as the issues of protein folding structure prediction. Further, since protein-ligand interactions are dynamic and complex; the issue of capturing these molecular movements over relatively long periods of time can be a great challenge. With the advent of advanced supercomputers and the development of algorithms, these challenges have been met in course of time.

Chapter 9, "Role of Supercomputers in Bioinformatics," by Anamika Singh, Rajeev Singh, and Neha Gupta, discusses supercomputing in sequence analysis, virtual screening, Quantitative Structure-Activity Relationship (QSAR), macro-molecular docking studies, micro-array data analysis, and applications of DNA microarray technology. Software and Web-based programs used for sequence analysis area also discussed.

Chapter 10, "Energy Network Operation in the Supercomputing Era," by Tianxing Cai and Neha Gupta has the objective to help the reader understand the idea of the applications of advanced computing techniques, especially for high performance and cloud computing technique applications in the energy network operation. The included application demonstration of environment protection and energy recovery are just the references for the readers. The real application can be extended but not limited to the above-mentioned topics. The technique significance and application demonstration have been presented in this chapter in order to attract more engineers, scientists, researchers, and the other related stakeholders to dedicate to the future research of this field.

Section 3 consists of four chapters on "Supercomputing Theory."

Chapter 11 "Steganography Encoding as Inverse Data Mining," by Dan Ophir, presents an introduction on the picture of steganography and its applications and historical development, and its linkage with cloud architectures and supercomputers, and other alternatives to supercomputers such as nCUBE, which is the machine's ability to build an order-ten hypercube supporting 1024 CPUs in a single machine.

This chapter also discusses that supercomputers do not have to oppose cloud computing. They both can become an integrated entity where the cloud-computing methodology is superimposed onto supercomputers. The beginning of this chapter alludes to the apparent competition between the two paradigms of supercomputing and cloud computing. The author of this chapter indicates that in the future the strengths of both systems will undergo a complementary integration, exploiting the powerfulness of the supercomputers and optimally using their idle time.

Chapter 12, "Cloud Computing: Future of the Past," by Manzoor Ahmed Khan and Fikret Sivrikaya, discusses basic concepts and motivation to use cloud computing, traditional cloud computing architectures of distributed storage architectures, computational services, higher infrastructure services, and mobile cloud computing architecture. This chapter introduced the concept of cloud computing, its components, applications, and architectural aspects. It also provides an overview of the stakeholders in the cloud market, with their corresponding perspectives to cloud computing. Software-Defined Networking (SDN) and Network Function Virtualization (NFV) concepts are covered as related technologies and enablers for both realization and utilization of cloud computing.

Chapter 13, "Programming Paradigms in High Performance Computing," by Venkat N. Gudivada, Jagadeesh Nandigam, and Jordan Paris, provides a fairly comprehensive introduction to various programming paradigms used in high-performance computing. Each paradigm is illustrated with a concrete programming example. The programs were chosen to illustrate the fundamental concepts of the paradigms rather than to demonstrate their esoteric or advanced features. The reader should consult the bibliography and additional resources sections for advanced and comprehensive exposition to the topics.

Chapter 14, "Data Mining for High Performance Computing," by Shen Lu, discusses how to use High-Performance Computing (HPC) in data mining. The basic concepts of data mining are discussed and several data mining algorithms are tested in a high-performance computing environment. In order to perform data mining on high-performance computing, several high-performance computing technologies need to be adjusted, such as process management, naming mechanism, message passing, remote procedure calls, distributed shared memory, and synchronization. Existing data-mining algorithms can be used in high-performance computing environments after choosing the proper mechanisms.

Experiments in this chapter used supercomputer Lonestar Server from the Extreme Science and Engineering Discovery Environment (XSEDE) Computing Center at Texas Advanced Computing Center (TACC) to do experiments. The Extreme Science and Engineering Discovery Environment (XSEDE) is the most powerful and robust collection of integrated advanced digital resources and services in the world. It is a single virtual system that scientists can use to interactively share computing resources, data, and expertise.

Lonestar is a Dell Linux Cluster, a powerful, multi-use cyberinfrastructure High-Performance Computer (HPC) and remote visualization resource. Lonestar is intended primarily for parallel applications scalable to thousands of cores so that normal batch queues will enable users to run simulations up to 24 hours. Experiments performed as shown in this chapter were for testing 7 data mining algorithms on a large lymphoma microarray gene expression data set with 240 instances and 522 attributes, and used several evaluation measurements to show the performance of each data-mining algorithm.

Section 4 consists of three chapters on "Supercomputing Leadership and Philosophy."

Chapter 15, "Super Leaders: Supercomputing Leadership for the Future," by Kim Grover-Haskin, discusses that the latest EDUCAUSE Center for Analysis and Research (ECAR) report on research computing states explicitly the need for collaboration between IT and faculty to perpetuate a dynamic environment for supercomputing to thrive in academia. Recommendations include developing research computing services infrastructure with researchers on grants, partner with other institutions, provide research staffing personnel, and be proactive in uncovering research computing needs.

If IT leadership recognizes the value of computational research, potential demand for research intensive study and support emerges for consideration. The strength of the vision relies on partnership and relationship, fundamental transformational leadership attributes most notable of women's leadership styles. Tomorrow's supercomputing leadership faces no shortage of talent. The challenge to the leadership is in preparing its future, readying a diverse, gendered, and global community of leaders for supercomputing.

Chapter 16, "Supercomputers: A Philosophical Perspective," by Jeremy Horne, discusses a supercomputer as thinking organism. This chapter provides somewhat of an overview of how supercomputer technological development may apply in recreating the human mind-brain, and also focuses on provoking discussion about emergence in an artificial brain by interweaving ideas somewhat repetitive but in different contexts. In other words, it is not the fascination of a brain's construction and how the architecture of a supercomputer might be mapped to it that is the focal point here but the implications. Neuroimaging advances and nanotechnology are two areas that may make at least a physical replication possible. The principle issue in producing a fully functioning brain is knowing precisely what the supercomputer will emulate, and what we think is a mind, thinking, and consciousness. Many times it is safer just to ask the question, but one cannot act on questions. When we find the answer we must be prepared for more dramatic problems, such as those concerning policy.

Chapter 17, "Supercomputers: A Philosophy of Their Language," by Jeremy Horne, explores the idea that binary logic as both a structure and the processes within it is innate in the universe. That is, what we set forth on paper as binary logic describes the essence of the universe. At its most fundamental level, it is a two-valued system, and binary logic displays all that happens with these values. The substance of the system may at first not appear to be elegant, but there appears to be an irreducible empirical truth in what constitutes order and how it translates into mind. The most immediate technical aspect of interfacing with a supercomputer is the language by which a supercomputer communicates: binary logic. The supercomputer has a potential of being a sentient entity.

All chapters went through a blind refereeing process at the initial phase, and then revised manuscripts were reviewed multiple times by the editor before final acceptance.

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Section 1

Overview to Global Supercomputing and its Current Challenges

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