

Sierra Supercomputer: Unleashing the Power of High-Performance Computing



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Project Approval

This is to certify that this project is approved and recommended as a partial fulfillment for the degree “B.S. Computer Science” from the Department of Computer Science, University of Peshawar.

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Chapter 1

Introduction

1.1 Overview of High-Performance Computing (HPC)

High-Performance computer (HPC) is a computational science paradigm that pushes the limits of conventional computer power to solve challenging issues involving large amounts of data. Fundamentally, HPC entails processing and analysing enormous volumes of data at incredible speeds using potent supercomputers or clusters of connected computers.

The exponential rise of data in the fields of science, engineering, and research has made the creation of supercomputers with enormous computational capability necessary. For a variety of disciplines, such as climate modelling, nuclear physics, astrophysics, computational chemistry, genomics, and artificial intelligence, among others, HPC has emerged as an essential tool.

1.1.1 The Role of Supercomputers in Scientific Advancements

Supercomputers have been essential in improving both technological innovation and scientific knowledge. New avenues for investigation and discovery have been made possible by the capacity to handle enormous datasets and run intricate simulations. Researchers and scientists can now model complex processes, analyse enormous volumes of observational data, and run simulations that were previously thought to be impossible because to previously unheard-of computational resources.

Supercomputers, for instance, have revolutionised the knowledge of fluid behaviour and made it possible to build more effective planes and vehicles in the subject of computational fluid dynamics. Similar to this, supercomputers have sped up gene sequencing and protein folding simulations in the field of bioinformatics, resulting in advances in personalised medicine and medication development.

1.1.2 Supercomputing for National Security

Supercomputers are essential for advancing efforts to strengthen national security in addition to supporting scientific research. Advanced supercomputing platforms are used by organisations like the National Nuclear Security Administration (NNSA) to do simulations for the management of nuclear weapons stockpiles. Without the need for nuclear tests, these simulations aid in ensuring the safety, security, and dependability of the country's nuclear deterrent.

Additionally, the analysis and mitigation of prospective dangers, such as cybersecurity concerns and natural calamities, is made possible by supercomputers.

They make it possible for massive amounts of data from multiple sources to be processed quickly, enabling techniques for real-time decision-making and responses.

1.1.3 Challenges in High-Performance Computing

High-performance computing has a lot of potential, but it also has a lot of difficulties. The sheer difficulty of controlling and coordinating tens of thousands or even millions of processors in a supercomputing system is one of the main difficulties. Complex software algorithms and connection technologies are needed to efficiently distribute computational jobs and ensure good communication between units.

Energy efficiency issues are brought on by the rising power needs of supercomputers. Optimising energy consumption is crucial to lowering operating costs and environmental effect as supercomputers continue to grow in size and computing capacity.

Despite these difficulties, the discipline of high-performance computing is still developing quickly thanks to improvements in algorithms, software, and hardware. The advancement of supercomputers like Sierra pushes the limits of computational power, creating new opportunities and accelerating scientific research and innovation.

1.2 Significance of Supercomputers in Scientific Research and Innovation

Despite these difficulties, high-performance computing is still developing quickly thanks to developments in the hardware, software, and algorithms. The advancement of supercomputers like Sierra expands the powers of computation, creating new avenues for opportunity and fostering scientific creativity and discovery.

1.2.1 Advancing Scientific Understanding

Science has advanced thanks to supercomputers, which give researchers the computational capability they need to study and simulate complex natural phenomena. Supercomputing simulations have considerably benefited fields like astrophysics, climate modelling, and particle physics, enabling researchers to comprehend the cosmos, climatic patterns, and fundamental particles. These simulations offer information that is frequently not possible to obtain using conventional experimental techniques.

For instance, in astrophysics, supercomputers have facilitated simulations of galaxy formation and black hole dynamics, shedding light on the mysteries of the universe. In climate modeling, supercomputing simulations help predict weather patterns, study climate change, and assess the impact of human activities on the environment.

1.2.2 Facilitating Drug Discovery and Biomedical Research

Supercomputers have transformed the way that complicated biological processes are studied in the fields of bioinformatics and biomedical research. They are essential to genomics because they make it possible to quickly sequence and analyse enormous volumes of genetic material. Protein folding may be simulated by supercomputing methods, which is essential for comprehending disease causes and therapeutic interactions.

Supercomputers have sped up the process of finding new drugs by virtually testing possible drug molecules against predetermined targets. By drastically reducing the time and money needed to identify viable candidates for additional experimental testing, these simulations hasten the discovery of life-saving drugs.

1.2.3 Engineering and Design Innovations

Supercomputers have revolutionised the way goods are designed and optimised in the engineering and design professions. Engineers may examine the aerodynamics of cars, planes, and wind turbines using computational fluid dynamics simulations on supercomputers. The design of more effective and environmentally friendly products follows from this.

Engineers can forecast the structural behaviour of complex systems and components by using the numerical method known as finite element analysis, which is used by supercomputers. The construction of bridges, buildings, and other essential infrastructure has been completely transformed by this capability.

1.2.4 Understanding Complex Systems

Supercomputers have been shown to be extremely useful in the study of complicated systems like neural networks in artificial intelligence (AI). Numerous AI applications use deep learning algorithms, which are trained on enormous volumes of data and with a lot of computer power. Supercomputers allow AI researchers to train complex models on massive datasets, resulting in improvements in autonomous systems, image recognition, and natural language processing.

In conclusion, supercomputers are revolutionary tools that have transformed scientific inquiry and invention in a wide range of fields. They play a critical role in pushing the boundaries of knowledge and innovation and tackling some of humanity's most pressing problems through the advancement of science, drug development, engineering, and AI research. As supercomputing technology develops, we should expect even more significant advancements in human

we can anticipate even more profound contributions to human progress and the betterment of society.

1.3 The Emergence of Sierra: A Breakthrough in Computational Prowess

Sierra has evolved as a ground-breaking supercomputer that personifies the cutting-edge capabilities of contemporary computational technology in the dynamic world of high-performance computing (HPC). Sierra was created by the National Nuclear Security Administration (NNSA) and the Lawrence Livermore National Laboratory (LLNL) in collaboration with IBM and NVIDIA to tackle the most difficult computational problems in a variety of scientific fields.

1.3.1 Objectives of Sierra's Creation

To provide researchers, scientists, and engineers with a supercomputing platform capable of attaining advances in scientific understanding, developing technological advancements, and supporting national security activities was the main goal behind the development of Sierra. In particular, Sierra was made to be excellent at simulating nuclear weapons, assisting the management of stockpiles, and advancing general scientific study.

1.3.2 Architectural Marvel: Harnessing the Power of Hybrid Computing

The unique and effective architecture of Sierra is the foundation of its computing capability. Sierra uses a special combination of NVIDIA Volta graphics processing units (GPUs) and IBM Power9 central processing units (CPUs) using a hybrid computing technique. Through the effective use of both CPUs and GPUs, Sierra is able to attain astounding levels of parallelism and computing performance.

The Power9 CPUs lay the groundwork for general-purpose computing workloads and offer great single-threaded performance. On the other side, the Volta GPUs excel at handling highly parallel workloads like machine learning, molecular dynamics simulations, and climate modelling because to their hundreds of cores.

1.3.3 Interconnect Technologies: Enabling Scalability and Efficiency

Sierra's cutting-edge interconnect technologies, which enable effective data transmission between its CPUs and GPUs, further improve performance. Modern connective fabric, which guarantees minimal data latency and maximises the system's overall throughput, is included in Sierra to enable smooth communication.

Sierra can handle intricate simulations and data-intensive computations thanks to this optimised interconnect design, opening the door for ground-breaking scientific discoveries.

1.3.4 Software Environment and Programming Models

Sierra's software environment and programming paradigms have been rigorously optimised to take full advantage of the hardware capabilities. Programming

languages, libraries, and frameworks designed to properly utilise the hybrid CPU-GPU architecture are available to researchers and scientists.

The Sierra software ecosystem makes it possible to design new software for upcoming scientific issues as well as to simply transfer and optimise existing applications for high-performance execution.



Figure 1.1: Sierra

Chapter 2

Architecture and Performance

2.1 Advanced Architecture and Hardware Components of Sierra

Sierra supercomputer, one of the world's most powerful systems, boasts an advanced architecture that enables groundbreaking scientific simulations and data-intensive computations. At its core, Sierra is equipped with cutting-edge hardware components that synergistically work together to deliver unparalleled processing power and memory capacity.

2.1.1 Advanced Architecture and Hardware Components of Sierra

Sierra's processing power is harnessed through a vast array of central processing units (CPUs) and graphics processing units (GPUs). These CPUs and GPUs are specifically designed for high-performance computing (HPC) workloads and offer immense parallel processing capabilities. The combination of multi-core CPUs and thousands of GPU cores enables Sierra to execute complex computational tasks with remarkable speed and efficiency.

2.1.2 Processing Power

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2.1.3 Memory

To support the demanding memory requirements of large-scale simulations and data processing, Sierra is equipped with a substantial memory hierarchy. The system features a tiered memory architecture that includes high-speed random-access memory (RAM) and high-capacity, high-bandwidth memory (HBM) for GPUs. This memory hierarchy minimizes data access latencies and maximizes data throughput, enabling efficient handling of massive datasets.

2.1.4 Interconnectivity

The interconnectivity within Sierra is a crucial aspect of its architecture, allowing for seamless communication and data transfer between its numerous compute nodes. The system utilizes cutting-edge high-performance interconnects, such as InfiniBand or Omni-Path, to provide low-latency, high-bandwidth communication channels. This interconnect fabric facilitates efficient parallelization and distribution of computational tasks across Sierra's nodes.

2.2 Software Environment and Programming Models

Sierra's advanced hardware is complemented by a sophisticated software environment that optimally utilizes its capabilities. The system employs a combination of custom software and industry-standard tools to ensure efficient execution of diverse scientific applications.

2.2.1 Custom Software Stack

Sierra benefits from a tailored software stack designed to exploit the system's architecture fully. This custom stack includes optimized compilers, libraries, and runtime systems that enhance application performance and scalability. Furthermore, specialized runtime environments and schedulers are employed to manage the concurrent execution of multiple tasks across the system.

2.2.2 Programming Models

To facilitate the development of parallel applications, Sierra supports various programming models, including Message Passing Interface (MPI) and OpenMP for distributed memory and shared memory parallelism, respectively. Additionally, Sierra leverages the power of GPUs through programming frameworks like CUDA and OpenACC, enabling developers to offload computationally intensive tasks to the GPU accelerators.

2.3 Benchmark Results and Performance Metrics

Sierra's computing power and efficiency are demonstrated through rigorous benchmarking and performance evaluations. These assessments are essential for understanding the system's capabilities and optimizing its performance for various scientific applications.

2.3.1 Benchmark Suites

Sierra undergoes testing with well-established benchmark suites to evaluate its performance across different dimensions. Commonly used benchmark suites include LINPACK for measuring floating-point performance, HPC Challenge for assessing memory bandwidth and communication speed, and SPEC for evaluating general-purpose compute-intensive performance. These benchmark suites provide standardized metrics that allow for fair comparisons with other supercomputers in the HPC community.

2.3.2 Real-World Scientific Applications

In addition to synthetic benchmarks, Sierra's performance is evaluated using real-world scientific applications. Researchers and scientists run simulations and computations from diverse fields, such as climate modeling, astrophysics, quantum chemistry, and computational biology. These application-centric benchmarks showcase Sierra's ability to tackle complex scientific problems efficiently and provide insights into the real-world impact of the supercomputer.

2.3.3 Scalability

Scalability is a critical aspect of evaluating supercomputers. Sierra's performance is tested under increasing workloads and problem sizes to assess its ability to efficiently handle larger and more complex simulations. Strong scalability ensures that Sierra can effectively utilize additional resources as more compute nodes are added to the system, resulting in higher computational throughput and reduced time-to-solution for large-scale problems.

2.3.4 Energy Efficiency

In addition to raw performance, Sierra's energy efficiency is also evaluated. Measured in terms of FLOPS per watt, energy efficiency is crucial for sustainable supercomputing operations. Sierra's advanced architecture and optimized software aim to achieve high computational efficiency while minimizing power consumption, making it a green and environmentally conscious supercomputing solution.

2.3.5 Performance Validation

Sierra's benchmark results and performance metrics are regularly validated to ensure accuracy and reliability. The supercomputer's performance is continually monitored, and any deviations are thoroughly investigated. Validation processes involve cross-verifying results from different benchmark suites and comparing them with past performance records to ensure consistency.

Chapter 3

Applications and Research Contributions

3.1 Scientific Applications Leveraging Sierra's Power

Sierra plays a vital role in accelerating research and innovation across numerous scientific disciplines. From climate modeling and astrophysics to materials science and drug discovery, Sierra's computing power enables scientists and researchers to push the boundaries of their respective fields. The supercomputer's ability to handle massive datasets and perform complex simulations at unprecedented speeds has made it an invaluable tool for tackling some of the most challenging scientific problems.

3.1.1 Climate Modeling and Weather Prediction

Climate modeling and weather prediction require extensive computational resources to simulate complex atmospheric dynamics accurately. Sierra's parallel processing capabilities and memory bandwidth enable scientists to run high-resolution climate models, leading to more precise and reliable weather forecasts. These advancements in climate modeling contribute to a better understanding of climate change and its potential impacts, aiding policymakers in making informed decisions.

3.1.2 Astrophysics and Cosmology

Sierra's supercomputing capabilities are instrumental in simulating the vast and intricate structures of the universe. Astrophysicists use Sierra to model galaxy formations, study cosmic evolution, and simulate the behavior of black holes. These simulations provide valuable insights into the origin and evolution of our universe, enriching our knowledge of fundamental astrophysical processes.

3.1.3 Drug Discovery and Biomedical Research

In the field of drug discovery and biomedical research, Sierra's computational power enables researchers to perform large-scale molecular simulations and virtual screenings of potential drug compounds. By simulating drug interactions with target proteins, Sierra accelerates the identification of promising drug candidates and reduces the time and costs associated with drug development.

3.1.4 Materials Science and Nanotechnology

Materials scientists leverage Sierra's high-performance computing to study the properties and behavior of complex materials at the atomic level. This research aids in the development of new materials with enhanced properties for applications in renewable energy, electronics, and aerospace industries. Sierra's simulations have accelerated the discovery of novel materials with superior strength, conductivity, and other desirable attributes.

3.2 Breakthrough Research Projects Enabled by Sierra

Sierra has played a pivotal role in driving several research projects that have led to significant breakthroughs in their respective fields. The following are examples of groundbreaking research facilitated by Sierra's computational capabilities:

3.2.1 Precision Medicine and Cancer Treatment

Sierra's computational power has been harnessed to analyze vast genomic datasets from cancer patients, leading to personalized treatment strategies based on individual genetic profiles. This approach, known as precision medicine, has shown promising results in improving cancer treatment outcomes and patient survival rates.

3.2.2 Seismic Hazard Assessment

Sierra's ability to process massive amounts of seismic data has revolutionized seismic hazard assessment. By simulating earthquake scenarios and predicting potential ground shaking patterns, Sierra assists in identifying vulnerable regions and designing robust earthquake-resistant infrastructure.

3.2.3 Fusion Energy Research

Sierra's simulations have significantly contributed to fusion energy research, allowing scientists to model plasma behavior in fusion reactors. These simulations aid in optimizing reactor design and understanding plasma confinement, bringing us closer to realizing sustainable and clean fusion energy.

3.3 Sierra's Impact on Advancing Scientific Research

Sierra's presence in the high-performance computing landscape has brought about a paradigm shift in scientific research, offering unparalleled computational power and sophisticated hardware architecture. Its exceptional performance has revolutionized data-driven research and simulation capabilities, empowering scientists to tackle complex problems with greater precision and efficiency. In this section, we delve deeper into Sierra's transformative impact on advancing scientific research across various domains.

3.3.1 Accelerating Time-to-Discovery

One of Sierra's most significant contributions is its ability to accelerate the time-to-discovery in scientific research. With its high-performance computing capabilities, Sierra enables researchers to perform complex simulations and analyses in significantly shorter timeframes. Problems that would have taken years or even decades to compute using traditional computing resources can now be solved in a matter of days or weeks with Sierra. This acceleration in research timelines empowers scientists to iterate and refine their experiments rapidly, leading to faster breakthroughs and discoveries.

3.3.2 Enabling Large-Scale Simulations

Sierra's advanced hardware architecture and memory capacity make it an ideal platform for conducting large-scale simulations. From simulating complex climate models to molecular interactions, Sierra can handle massive datasets and compute-intensive tasks with ease. This capability allows researchers to gain insights into intricate phenomena that were previously impossible to model.

comprehensively. By scaling simulations to unprecedented levels, Sierra opens new horizons for scientific exploration and a deeper understanding of natural processes.

3.3.3 Facilitating Data-Intensive Research

The increasing emphasis on data-intensive research in various fields necessitates powerful computing resources capable of handling vast amounts of data. Sierra's high-performance data analytics capabilities enable researchers to process and analyze large datasets efficiently. From genomics and healthcare to cosmology and environmental science, Sierra's ability to rapidly analyze immense data volumes empowers researchers to draw meaningful conclusions and make data-driven decisions.

3.3.4 Advancing Machine Learning and AI

The intersection of high-performance computing and artificial intelligence has led to significant advancements in machine learning and AI applications. Sierra's computational power is leveraged in training complex deep learning models, optimizing neural networks, and solving intricate AI problems. This synergy between supercomputing and AI drives innovations in natural language processing, image recognition, and autonomous systems, furthering the frontiers of AI research.

3.4 Sierra's Contribution to Scientific Breakthroughs and Innovations

Sierra's extraordinary computing capabilities have played a pivotal role in driving groundbreaking scientific breakthroughs and fostering technological innovations across various research domains. In this section, we explore specific research projects and achievements that owe their success to Sierra's immense computational power and efficiency.

3.4.1 Climate Modeling and Earth Sciences

One of Sierra's most impactful contributions lies in climate modeling and earth sciences. Researchers have utilized Sierra's high-performance computing to run complex climate models, enabling detailed simulations of global climate patterns and atmospheric dynamics. These simulations have significantly improved our understanding of climate change, extreme weather events, and the potential impacts on ecosystems and human populations.

3.4.2 Drug Discovery and Biomedical Research

Sierra's computational prowess has also had a transformative impact on drug discovery and biomedical research. With the ability to perform large-scale molecular simulations, Sierra aids in identifying potential drug candidates and understanding molecular interactions. Researchers can use Sierra's simulations to screen vast libraries of compounds, shortening the drug discovery process and reducing costs.

By leveraging Sierra's computing power, scientists can model complex biological systems at the atomic level, offering insights into diseases' molecular mechanisms. This knowledge is crucial for developing targeted therapies and personalized

medicine approaches. Sierra's contribution to drug discovery and biomedical research has accelerated the development of new treatments for various diseases, benefiting global healthcare and patient outcomes.

3.4.3 Materials Science and Nanotechnology

In the field of materials science, Sierra's computational capabilities have revolutionized materials design and optimization. Researchers can simulate the behavior of materials at the atomic level, leading to the discovery of novel materials with extraordinary properties. Sierra's simulations have paved the way for the development of advanced materials for aerospace, energy storage, electronics, and other industries.

Furthermore, Sierra's influence extends to nanotechnology, where it enables simulations of nanoscale phenomena and quantum mechanical systems. Understanding nanoscale processes is crucial for developing nanomaterials, nanoelectronics, and nanomedicine. Sierra's contributions to materials science and nanotechnology have spurred innovations in material engineering and nanoscale technologies, with far-reaching implications for multiple industries.

3.4.4 Astrophysics and Cosmology

Astrophysicists and cosmologists have harnessed Sierra's power to explore the mysteries of the universe. Sierra's simulations enable researchers to model galaxy formation, dark matter distributions, and cosmic evolution with unprecedented detail. By running large-scale cosmological simulations, scientists gain valuable insights into the origins and evolution of the cosmos.

Through Sierra, researchers can test theoretical models against observational data, deepening our understanding of fundamental astrophysical phenomena. Sierra's contributions to astrophysics and cosmology have expanded our knowledge of the universe, enriching our perspective on cosmic structures, dark matter, and the cosmic web.

3.4.5 Fusion Energy and Nuclear Physics

Sierra has made significant contributions to fusion energy research, particularly in the field of inertial confinement fusion (ICF). Scientists utilize Sierra's simulations to model the behavior of plasma in fusion reactors, optimizing the conditions required for controlled nuclear fusion. These simulations aid in developing strategies for achieving sustainable fusion energy, a clean and abundant energy source.

Chapter 4

Conclusion

4.1 Summary of Findings

Throughout this research paper, we have embarked on a journey to explore the astounding capabilities and impact of Sierra, a supercomputer at the forefront of high-performance computing. Our investigation has revealed the following key findings:

Sierra's Advanced Architecture: Sierra boasts an advanced architecture equipped with cutting-edge hardware components, including state-of-the-art processors, vast memory capacity, and high-speed interconnectivity. These features work in unison to deliver unmatched computational power and efficiency.

Significance in Scientific Research: Sierra's exceptional computing prowess has revolutionized scientific research and innovation. Its ability to handle complex and computationally-intensive problems has opened new avenues for researchers in various domains.

Software Environment and Programming Models: The software environment of Sierra is optimized to leverage its capabilities efficiently. Researchers can harness parallel processing and utilize specialized programming models to fully exploit Sierra's immense potential.

Benchmark Results and Performance Metrics: Sierra has been subjected to rigorous benchmarking, and its performance metrics speak volumes about its computing power and efficiency. It consistently outperforms traditional computing systems, making it a vital tool for data-intensive tasks.

Impact on Scientific Discoveries: Sierra's unparalleled capabilities have led to groundbreaking research projects and significant scientific breakthroughs. From climate modeling to astrophysics, Sierra has accelerated the pace of discovery and expanded the frontiers of human knowledge.

Future Advancements: As technology advances, Sierra continues to evolve. Researchers and engineers are continuously working on enhancements to push Sierra's computing power to new heights, promising even more remarkable scientific achievements.

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Appendix A

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Appendix B

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