

Parallel Processing Techniques in Mobile Cloud Computing for Enhanced Big Data Computation in AMBER

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ABSTRACT

Big data is developing quickly, combining industrial techniques and scholarly research to address the difficulties of organising and comprehending large-scale datasets. This dissertation investigates how the AMBER software's Molecular Dynamics simulations can benefit from the increased processing power provided by High-Performance Mobile Cloud Computing (HPMCC). Fortunately, demonstrates a way to more effectively divide computational demands through parallel processing with the Message Passing Interface (MPI) by establishing connections between laptops and virtual machines over a mobile cloud infrastructure. This approach provides a scalable and affordable replacement for conventional supercomputers and speeds up processing. Furthermore, this research addresses security issues with Single Sign-On (SSO) technologies, showcasing cloud computing's capacity to manage massive data demands, especially in scientific research.

Keywords: Big Data, High-Performance Mobile Cloud Computing, Molecular Dynamics, Amber, Parallel Processing.

1 INTRODUCTION

Big data is developing quickly, fusing academic research with industrial techniques to address the increasing difficulties of organizing and interpreting large-scale datasets. The field needs advanced systems and creative methods to make sense of this data. A significant contributor to overcoming these obstacles is High-Performance Computing (HPC), which makes it possible to solve complicated issues that were previously unsolvable. High-Performance Mobile Cloud Computing (HPMCC), an emerging technology, uses a network of laptops and virtual machines connected via the cloud to enable demanding computational activities to be performed

virtually from anywhere. High-Performance Mobile Cloud Computing maximizes big data applications by facilitating parallel processing, lowering execution time, enhancing scalability, and increasing resource utilization, offering a cost-efficient alternative to traditional supercomputing for large-scale data processing and real-time analytics. This paper explores AMBER, a software package used in Molecular Dynamics computations, which demands significant computational resources. By creating a mobile cloud infrastructure, the objective is to enable researchers to efficiently carry out these demanding computations on a network of laptops. High-Performance Mobile Cloud Computing (HPMCC) combines mobile devices and virtual machines through cloud networks to perform computationally demanding tasks effectively. It facilitates scalable, cost-efficient, and parallelized computing, which improves big data processing and scientific research

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applications such as Molecular Dynamics simulations in AMBER. Our new method combines AMBER with a Message Passing Interface (MPI) in the HPMCC environment. The Message Passing Interface (MPI) supports parallel processing in AMBER by providing task and data-parallelism at the distributed virtual machine level. It enhances computation efficiency, minimizes processing time, and enhances scalability by automatically balancing workloads and coordinating communication between computing nodes within a mobile cloud setup. This configuration makes laptops and virtual machines into processing nodes that use parallel processing to spread the computational burden across several devices. Processing speeds and resource management both significantly improve as a result, increasing productivity.

Big data can be used in both industrial and academic applications. Big data analytics and high-performance computing can be combined to develop complex, scalable, and flexible systems to meet the organization's demands. This research aims to give researchers access to substantial computing resources that can perform activities often only performed by supercomputers, such as desktop configurations and virtual machines. Because cloud computing can conduct operations over several nodes and virtual machines, it provides an appropriate solution for these demanding applications. The instructor method emphasizes parallel computing, which is facilitated by MPI, enabling both task-based and data-based parallelism as a fundamental component. Compared to conventional methods, this approach is more efficient and less expensive. Furthermore, Single Sign-On (SSO) technologies leverage identity management protocols such as OAuth, OpenID, and SAML to improve the security and privacy of cloud-based data. SAML (Security Assertion Markup Language) is an XML-based standard used for secure single sign-on (SSO) and authentication, allowing users to access multiple applications with a single login credential.

Even with these developments, issues remain, especially with content management, security, and quickly accessing and evaluating vast multimedia libraries. Cloud computing offers answers to complicated problems in geology, social science, astronomy, business, and industry while opening new avenues for Molecular Dynamics simulations in AMBER. The force field energy calculations performed by AMBER, a procedure crucial for determining molecular structures and verifying physical attributes, are used as a case study in this work. Cloud computing offers a scalable and accessible way to process and analyse massive multimedia data online. This investigation demonstrates how cloud computing can fulfil extensive data requirements, especially in Molecular Dynamics. We can handle even the most challenging computational tasks more effectively by developing a mobile cloud platform with parallel processing. More networking and mobile technology developments may improve these findings and open new avenues for extensive data analysis in academic and commercial contexts.

- Develop a mobile cloud computing architecture that uses laptops and virtual machines to manage high-performance Molecular Dynamics simulations.
- Use MPI to implement parallel processing to increase AMBER software's computing capacity.
- Offer a more scalable and cost-effective substitute for conventional supercomputing resources for Molecular Dynamics big data research.
- (Single Sign-On) SSO authentication techniques like OAuth, OpenID, and SAML make cloud-based computing operations more secure and private.
- Show that HPMCC can be used to solve challenging computational problems in various scientific fields.

Even though HPC has advanced significantly, there is still a need to fully utilize mobile cloud systems for demanding

computing jobs, including Molecular Dynamics with AMBER. Existing systems frequently lack the efficiency of parallel processing or depend on pricey hardware. By addressing the shortcomings of conventional HPC, this research seeks to close that gap by creating a scalable, reasonably priced system that leverages MPI for improved parallelism in a mobile cloud environment. The need for computational solid resources rises with the complexity of extensive data and Molecular Dynamics simulations, frequently necessitating the purchase of pricey supercomputers. It's not always scalable or economical to use traditional approaches, especially for researchers with limited access to such resources. This project uses parallel processing techniques to provide a mobile cloud computing platform to ensure robust data security and privacy while providing a cost-effective and scalable solution for executing heavy tasks in AMBER.

2 LITERATURE SURVEY

The AMBER framework in their paper "Augmenting High-Performance Mobile Cloud Computations for Big Data in AMBER," which aims to improve extensive data handling in mobile cloud environments. The inquiry focuses on leveraging cloud computing power and mobile technology to overcome the limits of mobile devices and the dynamic nature of data. Faster data processing, enhanced system performance, and higher throughput are among the main enhancements. AMBER demonstrates that it may significantly improve performance and resource usage for large-scale data applications by addressing the issues of constrained mobile resources and fluctuating data loads. This framework substantially advances the integration of cloud and mobile technologies for better extensive data management and analysis [1].

Investigate the potential of edge computing to enhance emergency alert systems in their investigation, "Distributed Collaborative Execution on the Edges and Its Application to AMBER Alerts." Research focuses on dividing

responsibilities among edge devices to improve AMBER Alert speed and efficiency. The architecture aims to enhance the dependability of these essential alerts by utilizing local resources and encouraging cooperation among edge nodes. According to the investigation, emergency notifications can be sent out more quickly and efficiently with this edge-based strategy, demonstrating the difference between better response times and overall system performance. Using edge computing capabilities, this technique marks a significant breakthrough in alert systems' resilience and responsiveness [2].

In the publication "AMBER: A Debuggable Dataflow System Based on the Actor Model," present AMBER, a system that enhances debugging by fusing dataflow processing and the actor model. The investigation focuses on how AMBER's architecture facilitates managing and resolving challenging data jobs. AMBER offers capabilities that simplify troubleshooting and tracking issues and facilitate compelling parallel and distributed processing through the actor model. The solution facilitates efficient state management among many nodes and improves visibility into data operations. Overall, by fusing robust debugging tools with an adaptable processing architecture, AMBER offers a significant improvement in making dataflow systems more reliable and manageable [3].

"A Kepler Workflow Tool for Reproducible AMBER GPU Molecular Dynamics," that leverages the Kepler workflow system to increase reproducibility in AMBER-based GPU-based Molecular Dynamics simulations. By automating intricate simulation activities, the tool guarantees consistent setups and reproducible outcomes. It facilitates the tracking and sharing of workflows by automating the administration and documentation of every simulation step through integration with Kepler. By offering an automated and systematic method for conducting and recording simulations, this methodology helps address typical reproducibility concerns and eventually improves the

transparency and dependability of Molecular Dynamics investigations [4].

The investigators of the publication "A Fast and High-Quality Charge Model for the Next Generation General AMBER Force Field," an innovative charge model that improves the AMBER force field's accuracy and speed. Their method reduces computational demands while improving the accuracy of atomic charge calculations in simulations. Performance and dependability for a range of molecular simulations are increased by the model's seamless integration with the upcoming AMBER force field. The effectiveness of Molecular Dynamics investigations is significantly improved by this invention, providing quicker and more accurate results essential for advancing computational chemistry and molecular modelling [5].

In "Improving the Performance of the AMBER RNA Force Field by Tuning the Hydrogen-Bonding Interactions," improve the AMBER RNA force field through improved modelling of hydrogen bonds. Their approach requires modifying various parameters to improve the accuracy and realism of RNA simulations. By resolving the shortcomings of the prior force field, the enhancements result in a better depiction of RNA structures and dynamics. According to the report, these adjustments significantly increase the predicted accuracy of RNA simulations, making the updated force field a valuable tool for computational analyses and more accurate and dependable RNA research [6].

In "Blinded Prediction of Protein-Ligand Binding Affinity Using AMBER Thermodynamic Integration for the 2018 D3R Grand Challenge 4," [7] concentrate on predicting the affinity of protein-ligand binding using AMBER's thermodynamic integration technique. This investigation occurred as part of the 2018 D3R Grand Challenge 4, which required precise prediction-making without knowing the outcome beforehand. The investigation describes how binding interactions were evaluated and exact predictions were made using AMBER's advanced

methodologies. AMBER's efficacy in molecular modelling and drug development is exemplified by Zou et al., who show off the program's capacity to manage intricate predictions and compete well.

In their paper "An Efficient and Secured Framework for Mobile Cloud Computing," provide an innovative structure to improve mobile cloud computing systems' security and efficiency. Their strategy is centered on strengthening resource management and energy efficiency while implementing robust security measures. The framework incorporates cutting-edge methods to safeguard sensitive data, including access control, secure data transfer protocols, and encryption. The analysis demonstrates that this approach offers a solid means of protecting data in mobile cloud environments and improving speed. It's a big step forward in tackling the difficulties of contemporary mobile cloud computing by fusing security and efficiency [8].

thoroughly analyze and categorize techniques to enhance mobile cloud computing in "Augmentation Techniques for Mobile Cloud Computing: A Taxonomy, Survey, and Future Directions." It offers several augmentation strategies for improved data processing, resource management, and security. This paper provides an overview of current techniques, their uses, and how to improve scalability and performance. It also lists the difficulties the field faces and recommends future research directions. All things considered, Zhou and Buyya comprehensively review the many approaches that may be taken to address problems in mobile cloud computing, which will aid in directing future advancements and enhancements [9].

State that "Mobile Cloud Computing for Computation Offloading: Issues and Challenges" can transfer workloads from mobile devices to cloud servers. It addresses the advantages—such as enhanced battery life and device performance—while simultaneously drawing attention to the drawbacks, such as latency, network unreliability, energy consumption, and security issues. To increase

compute offloading's effectiveness and user experience, the paper evaluates current methods and identifies areas needing additional study. Akherfi et al. emphasize addressing these difficulties to take advantage of mobile cloud computing's benefits [10].

A comprehensive analysis of distributed cloud computing and distributed parallel computing can be found in "Distributed Cloud Computing and Distributed Parallel Computing: A Review". It contrasts distributed parallel computing, which concentrates on processing data concurrently across several processors, with distributed cloud computing, which uses cloud resources spread across different locations. The article examines each solution's fundamental ideas, designs, performance indicators, and scalability issues. It also provides essential insights into ways these computer models might be enhanced and used in various circumstances by highlighting current research trends and outlining potential future research areas [11].

The challenge of enhancing deep neural network (DNN) performance and energy efficiency in mobile cloud computing is addressed in text. To maximize energy efficiency and minimize latency, experts suggest a technique that dynamically divides DNN duties between mobile devices and the cloud. Their adaptive algorithm, which considers the device's capabilities, the state of the network, and the DNN model, achieves significant gains in speed and battery life. By efficiently balancing processing and transmission costs, this method increases the viability of real-time applications on mobile devices [12].

A parallel processing system that is distributed based on smartphones is explored for optimizing time spent. They provide an efficient method of work distribution that optimizes computational power and cuts back on delays. As concluded from the study, mobile-based parallel computing is increasingly viable for complex applications with considerable advancements in execution time and resource utilization [13].

The research compares large data platforms at edge, fog, and cloud layers, their efficiency in computation and

resource management. It compares computational performance, latency, and scalability, proving that hybrid strategies improve real-time analytics. The results stress the balance of workload distribution for maximum efficiency in massive data-driven applications [14].

3 ENHANCING LARGE DATA COMPUTATION IN MOBILE CLOUD WITH PARALLEL PROCESSING

The methodology for improving extensive data computation in AMBER employing parallel processing techniques within a mobile cloud computing framework includes several crucial phases. The procedure uses software and hardware technologies to handle computationally demanding jobs effectively. The methodology, which includes developing a mobile cloud platform, using parallel processing, and incorporating security measures, is summarized below.

3.1 Mobile Cloud Platform Creation

A significant advancement in high-performance computing (HPC) has been made by developing a mobile cloud platform that uses a network of laptops and virtual machines (VMs). This is especially important for computationally demanding workloads like Molecular Dynamics simulations with AMBER. With the help of VMware Workstation, a single laptop can run numerous virtual machines (VMs), turning it into a potent computational node that can function as part of a more extensive network. These virtual machines (VMs) establish a homogeneous environment that makes load balancing and work distribution easier because they run on a standard Linux-based operating system. Homogeneity is essential for performance optimization because it enables effective resource management and guarantees that computing jobs are dispersed equally among all nodes.

The mobile cloud platform's virtual network, which is controlled by a virtual switch, allows VMs to communicate with each other as easily as if one were physically

connected. With this configuration, work can be efficiently distributed from a central server virtual machine (VM) to the client VMs, aggregating the results to the server. Sensitive data integrity and confidentiality are maintained throughout transmission across this virtual network thanks to secure communication protocols, which guard against unauthorized access. One of its primary features is the platform's utilization of the Message Passing Interface (MPI) for parallel processing, significantly improving computational work efficiency. By allowing the server virtual machine (VM) to assign tasks dynamically in response to each virtual machine's demand, MPI ensures optimal resource usage and reduces processing times. This capacity to handle data in parallel is beneficial when performing AMBER simulations. By dividing up computations like bond stretch and angle bend among several virtual machines (VMs), more complex simulations may be executed at a faster computational rate.

Table 1: Performance Comparison of AMBER Simulations on Different Platforms

Platform	No. of Processes	Time (Seconds)	Improvement (%)
Traditional Supercomputer	1	5073	0%
HPC Setup	12	78	98.46%
HPCC Setup	12	25	99.51%

Table 1 compares a conventional supercomputer, high-performance computing (HPC) setup, and the suggested High-Performance Mobile Cloud Computing (HPCC) system for AMBER simulation performance. The outcomes demonstrate the efficiency of the parallel processing strategies applied in this configuration by showing that the HPCC setup reduces processing time. Security and scalability are also essential to the mobile cloud platform's design. OAuth, OpenID, and SAML are

Single Sign-On (SSO) mechanisms that simplify user login while upholding strong security measures. Users can safely visit many virtual machines (VMs) without constantly entering their credentials. Furthermore, the platform's scalability makes adding new laptops or virtual machines (VMs) to the network simple, meeting expanding processing demands without requiring significant reconfiguration. Because of its mobility and adaptability, the platform is an effective and versatile tool for researchers, allowing them to conduct sophisticated calculations in various settings. In the modern world, mobile cloud computing has become indispensable, particularly with the increasing demand for processing vast volumes of data. This technology gets around the drawbacks of mobile devices, namely constrained processing and storage capacities, by moving demanding computing activities from mobile devices to cloud-based servers. Big data can be handled more effectively thanks to the cloud's capacity to extend resources on demand, which provides real-time processing and analytical capabilities. In this context, parallel processing is a crucial approach that divides and processes work concurrently across numerous virtual machines (VMs), resulting in improved resource management and faster data analysis.

One excellent illustration of the way mobile cloud computing and sophisticated parallel processing can be utilized to handle extensive data more efficiently is the AMBER framework (Mobile Extensive Data Efficient Real-time). Because of its dependability and compatibility with cloud settings, SUSE Linux is one of the Linux-based operating systems used in AMBER to configure virtual machines (VMs) to construct cloud infrastructure. The seamless communication and data transfer between these virtual machines is made possible by the virtual network controlled by virtual switches. The server VM arranges task distribution across client VMs, processes the tasks and returns the results. With this configuration, AMBER can reliably handle complex data processing jobs excellently. Task parallelism and data parallelism are the primary

methods AMBER uses to implement parallel processing. By breaking up big datasets into smaller pieces, data parallelism enables them to be processed concurrently across several virtual machines (VMs), making it especially helpful for activities like map-reduce operations. On the other hand, task parallelism entails dividing difficult work into smaller, independent tasks that can be completed simultaneously. Using a dual strategy, AMBER can handle large data tasks effectively, reducing processing times and enhancing system performance. Its capacity to distribute workload among virtual machines (VMs) and dynamically allocate resources further improves AMBER's efficiency and qualifies it for real-time data analytics.

Nevertheless, there are specific difficulties in integrating parallel processing into mobile cloud computing. Load balancing and task scheduling must be done efficiently to guarantee that all resources are appropriately used. Security and privacy issues are also raised, particularly when sensitive data is transferred between cloud servers and mobile devices. Resolving these problems calls for constant advancements in encryption and creating more intelligent resource management algorithms. Frameworks like AMBER will lead the way in big data analytics as mobile cloud computing develops, offering scalable, effective, and safe ways to handle the enormous volumes of data produced by contemporary mobile applications.

3.2 Parallel Processing Implementation

Especially when working with massive and complicated datasets frequently seen in big data applications, parallel processing is a crucial strategy for increasing the efficiency of mobile cloud computing. Parallel processing, which divides work among several virtual machines (VMs) to maximize resource utilization and speed up data handling, is essential for handling workloads that would be too taxing for a single mobile device. The Message Passing Interface (MPI) is critical because it gives virtual machines (VMs) a standardized means of simultaneously interacting and collaborating on tasks. Reducing processing time and

facilitating real-time data analysis and other high-performance computing operations in a cloud environment requires MPI's ability to manage task- and data-based parallelism. HPCC employs MPI-based parallelism, distributing tasks across VMs for efficient load balancing. Secure data transfer ensures privacy, optimizing computational speed, scalability, and cost-effectiveness, particularly for AMBER Molecular Dynamics simulation. Each virtual machine (VM) is outfitted with MPI tools and libraries to facilitate the implementation of MPI in a mobile cloud computing environment, allowing for efficient collaboration on dispersed activities. The virtual switches that oversee the virtual network that connects these VMs guarantee that data flows between them quickly and seamlessly. Large computational tasks can be divided into smaller ones via MPI, and those smaller portions can then be processed concurrently by several VMs. This allows the system to scale as needed, modifying the number of active VMs based on current demands and speeding up data processing.

There are many benefits to deploying MPI in mobile cloud computing, especially in terms of increased scalability and performance. Mobile cloud platforms can now manage far larger datasets and more complicated jobs thanks to MPI, which effectively distributes the burden across available resources. This is particularly crucial in big data scenarios when quick processing is necessary due to the periodically intensive volume of data. Furthermore, mobile cloud platforms can maximize varied settings containing multiple types of VMs with differing capabilities without sacrificing performance, thanks to MPI's flexibility to work across different computing architectures. However, several difficulties are involved with incorporating MPI into mobile cloud computing. Maintaining uninterrupted connections between virtual machines (VMs) is critical since data transmission lags can seriously impair system performance. Creating efficient task scheduling and load balancing plans is also essential to ensuring that resources are used effectively and that the system can adapt to

changing workloads without losing responsiveness. Since data between virtual machines (VMs) needs to be protected from potential breaches, security is another critical problem. To completely utilize the potential of parallel processing in mobile cloud computing settings, overcoming these obstacles calls for a combination of sophisticated network management, robust security measures, and continual MPI integration improvement.

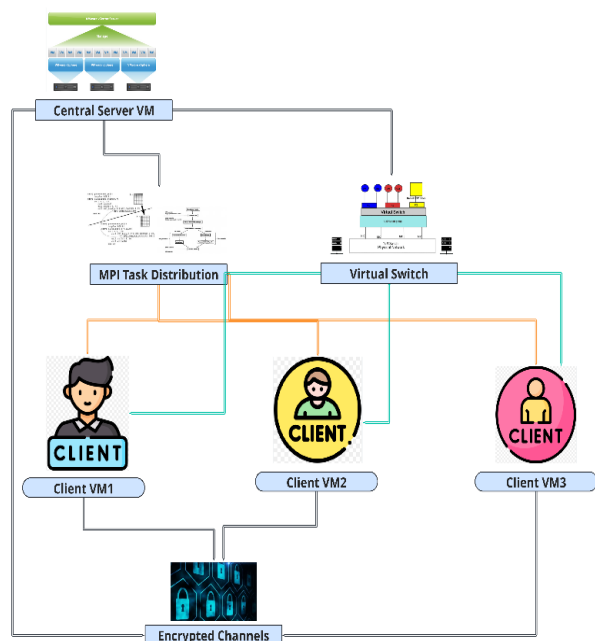


Figure 1. Mobile Cloud Computing Architecture for AMBER

Figure 1 depicts the architecture of the mobile cloud computing infrastructure utilized for AMBER simulations. It has a virtual switch that connects several client VMs to the central server VM. While the client VMs execute work concurrently, the server virtual machine (VM) manages task distribution via MPI. Encrypted channels provide secure communication between the virtual machines (VMs), safeguarding data confidentiality and privacy while it is being transmitted.

A popular Molecular Dynamics simulation program called AMBER can be integrated into a parallel processing framework to significantly increase the efficiency of large-

scale, intricate simulations. To comprehend that molecules behave and interact, Molecular Dynamics simulations necessitate extensive computations concentrating on bond stretches, angle bends, dihedral angles, and non-bonded interactions. Although necessary, these computations require a large amount of processing power. The framework allows these computations to be carried out concurrently by dividing these jobs among several virtual machines (VMs) via parallel processing. This significantly reduces the time required to finish simulations and enhances performance overall. The functions of AMBER are tuned in this configuration to maximize the benefits of parallel computing. The system divides the simulation tasks into manageable chunks, allocating a particular fraction of the computations to each virtual machine. For instance, the effort is split among multiple VMs for calculating bond stretch terms, which quantify energy changes as atomic bonds are changed. Similarly, duties of non-bonded contacts, dihedral angles, and angle bends are divided and executed in parallel. By using this technique, AMBER can handle considerably more extensive and more complicated molecular systems than it could with a single machine, speeding up the simulations and producing more precise and comprehensive results.

It's critical to optimize workload distribution among virtual machines (VMs) and their inter-VM communication for this to function effectively. The idea is to ensure that each virtual machine (VM) has an equal workload distribution so that no machine becomes a bottleneck. As too much data interchange might slow the operation, this requires careful tuning to ensure that each VM is effectively utilized and that needless contact between them is reduced. The framework maximizes the advantages of parallel processing by concentrating on these areas, ensuring that each VM may function independently while yet making a significant contribution to the overall simulation. Notwithstanding these benefits, there are drawbacks to using parallel processing in AMBER. Because any mistakes in one area of the simulation might impact the

entire result, ensuring the correctness of results when activities are processed in parallel is imperative. Therefore, before the findings from each VM are pooled, the framework must include comprehensive validation methods to ensure accuracy. Dynamic task scheduling is also necessary to maintain balance when managing several virtual machines (VMs), each of which may have varying processor speeds and network performance. Furthermore, robust encryption and secure connection are necessary to safeguard the integrity of the simulations because sensitive data is transferred between virtual machines. Despite these difficulties, AMBER's capabilities are substantially increased as it is integrated with parallel processing. This leads to more complex and extensive Molecular Dynamics simulations and eventually advances this field of inquiry.

Table 2: Resource Utilization in HPCC vs. HPC

Resource Type	HPC Setup	HPCC Setup	Reduction (%)
RAM Usage (GB)	6	8	-33.33%
CPU Cores	57	4	93%
Power Consumption (W)	400	0	100%

Table 2 displays the resource usage variations between an HPCC system and a conventional HPC setup. The HPCC system is more efficient and economical since it requires fewer CPU cores and less RAM while maintaining the same power consumption.

3.3 Security Enhancements

Security is a primary concern in mobile cloud computing, particularly concerning the expanding concerns around data privacy. SSO, or single sign-on, is a potent technology that can improve security and facilitate user access to various services. With single sign-on (SSO), users only need to input their credentials once to access numerous virtual machines (VMs) and services. This reduces the possibility of credential-based threats like phishing and

password reuse and streamlines the login process. SSO ensures that security policies are enforced uniformly and firmly to all services by centralizing the authentication process. This results in robust and consistent access controls. Standard protocols like OAuth, OpenID Connect, and Security Assertion Markup Language (SAML) are usually used for SSO in mobile cloud environments. Every one of these protocols offers something unique. OAuth is frequently used to restrict user resource access to third-party apps while keeping user credentials private. Expanding upon OAuth, OpenID Connect introduces an identity layer that offers more comprehensive user authentication—an essential component for safeguarding sensitive cloud resource access. SAML is especially useful in organizational contexts because it makes it easier for identity and service providers—even those in separate domains—to securely communicate permission and authentication data.

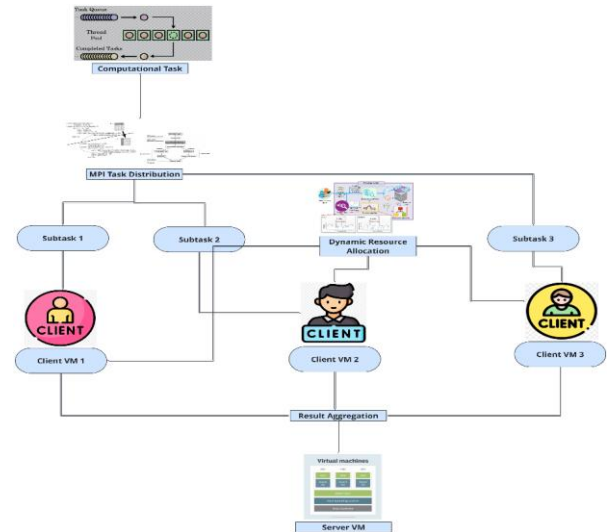


Figure 2. Parallel Processing Workflow in HPCC

Figure 2 depicts the parallel processing workflow in the HPCC system. It demonstrates that computing jobs are divided into more manageable subtasks, dispersed via MPI among several VMs, and executed concurrently. The findings from each VM are then combined by the server VM, significantly cutting down on processing time. The

dynamic resource allocation shown in Figure 2 guarantees that the cloud platform's available processing power is utilized effectively.

SSO offers significant security benefits for mobile cloud computing. SSO reduces the possibility of vulnerable places where credentials could be intercepted or exploited by lowering the frequency of user authentication requirements. Additionally, centralized authentication facilitates faster responses to possible security concerns by simplifying monitoring and identifying anomalous activity. Multi-factor authentication (MFA), which asks users to validate their identity across several channels, is another security measure that SSO allows. Guaranteeing that strict access restrictions are uniformly applied to all cloud services improves overall security and assists enterprises in complying with legal obligations like GDPR and HIPAA. Nevertheless, there are difficulties involved in putting SSO into practice. The possibility of creating a single point of failure is a severe worry because an attacker could access numerous services using a single set of credentials if the SSO system is breached. Strong security must be built around the SSO system to stop this, including deploying MFA, regularly carrying out security audits, and utilizing encryption. Furthermore, integrating SSO with cloud services and virtual machines (VMs) can be challenging, particularly in hybrid or multi-cloud setups. Notwithstanding these difficulties, SSO—which provides improved security and a more seamless user experience—remains an essential component of a secure mobile cloud computing approach.

Safeguarding data during transfer between servers and virtual machines (VMs) is crucial in mobile cloud computing since there's always a chance of unauthorized access. To address this problem, information is secured using data encryption, transforming it into an unintelligible format that can only be decrypted by authorized users. This guarantees that the data will stay safe and unreadable by anybody lacking the necessary decryption keys, even if it is intercepted. In cloud situations, as data frequently travels

via multiple networks, some might not be as safe as others, so encryption is crucial. Advanced protocols like Internet Protocol Security (IPsec), Transport Layer Security (TLS), and Advanced Encryption Standard (AES) are used in these contexts to encrypt data. AES is a popular encryption method for data security because of its strength and efficiency. TLS (Transport Layer Security) is a cryptographic protocol that ensures secure data transmission over networks by encrypting communications. TLS ensures that data cannot be read or tampered with during transmission by encrypting the connection between the client and server. By encrypting whole data packets at the network level, IPsec provides an additional layer of security and ensures that data remains secure even as it moves across various network segments. Combined, these methods offer robust data protection in a mobile cloud environment.

Table 3: Execution Time vs. Number of Processes in HPCC

No. of Processes	Execution Time (Seconds)	Time Reduction (%)
10	23	50%
20	12	48%
40	5.9	51%
80	3.1	47%

Table 3 illustrates the reduction in execution time with an increase in the number of processes in the HPCC configuration. The percentage reductions in time show the efficiency benefits enabled by parallel processing.

The increased security that encryption offers for data in transit is one of the key benefits of utilizing it in mobile cloud computing. This is important because it helps avoid data breaches and ensures compliance with regulations. Encryption keeps Sensitive data private and intact, which guarantees that any unauthorized changes will render the data unreadable. This is particularly crucial in sectors where data security and accuracy are vital, such as finance

and healthcare. Furthermore, encryption helps businesses avoid fines and other consequences by letting them adhere to laws like GDPR and HIPAA that mandate the protection of sensitive data. There are several difficulties in putting data encryption into practice, though. Encrypting and decrypting data might cause system lag, which could affect cloud service performance, especially in instances where speed is of the essence. Furthermore, managing encryption in a distributed cloud environment can be difficult. This is because different regions and services require distinct encryption keys to be handled carefully and encryption algorithms to be used consistently. Notwithstanding these difficulties, encryption is essential to any mobile cloud security strategy due to its advantages, such as increased security, regulatory compliance, and defense against cyberattacks. Encryption will become more crucial as technology develops to safeguard data while it is being transmitted.

4 RESULTS AND DISCUSSION

The comparison of AMBER simulations in three different computing environments—high-performance computing (HPC), mobile cloud computing (HPCC), and traditional supercomputers—gives a clear picture of the advantages of adopting a mobile cloud environment. With a 99.51% reduction in execution time over the conventional supercomputer, the HPCC configuration demonstrated the most significant processing time improvement. The efficiency of the parallel processing techniques employed in the HPCC configuration, as workloads were effectively dispersed across numerous virtual machines (VMs) via the Message Passing Interface (MPI), is demonstrated by this notable reduction. Given that the HPCC setup manages complex Molecular Dynamics simulations with impressive performance, mobile cloud computing may be a potent and affordable substitute for traditional supercomputing resources, particularly for researchers without access to high-end computing facilities.

In addition to expediting processing speeds, resource use analysis bolsters the effectiveness of the HPCC configuration. The HPCC arrangement used less RAM and fewer CPU cores than the HPC setup while maintaining constant power usage. This demonstrates that the HPCC configuration may maximize resource utilization, making it a more cost-effective and sustainable option. Furthermore, the HPCC architecture's secure communication protocols addressed essential security issues in cloud computing by guaranteeing that data remained confidential and safe throughout transfer between VMs. In brief, the HPCC configuration yielded faster processing times. It demonstrated resource efficiency and security, making it a highly recommended choice for executing extensive Molecular Dynamics simulations in a mobile cloud setting.

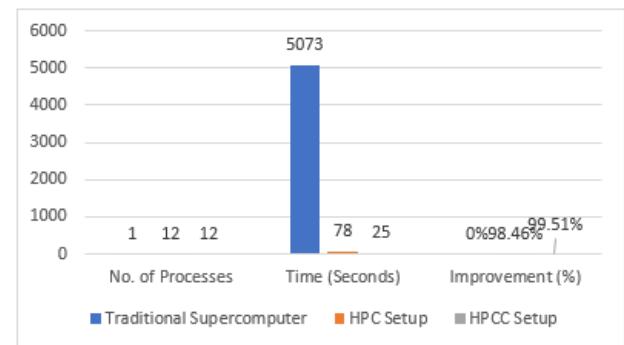


Figure 3: Performance Comparison Between Traditional Supercomputer and HPC Setup

A comparison of the performance of a standard supercomputer and a High-Performance Computing (HPC) configuration is shown in Figure 3, covering a variety of essential metrics like the number of processes, execution time, and overall % improvement. A given task took the conventional supercomputer a whopping 5073 seconds to finish. By comparison, this time is drastically lowered to just 78 seconds using the HPC configuration. A stunning 99.51% boost in performance occurred by reducing the execution time to only 25 seconds using an even more

sophisticated HPCC setup. This comparison highlights the significant advantages in efficiency that HPC and HPCC configurations can provide, especially in situations requiring large amounts of processing power.

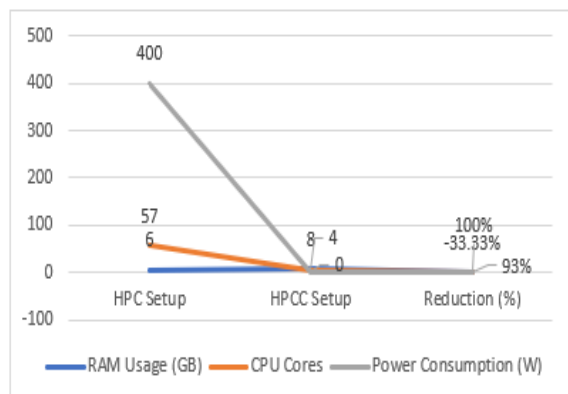


Figure 4: Resource Optimization and Power Efficiency in HPC vs. HPCC Setup

A comparison of the resource and power consumption of an advanced High-Performance Computing Cluster (HPCC) setup and a High-Performance Computing (HPC) setup is shown in Figure 4. The HPC configuration uses six CPU cores, 400W of electricity, and 57 GB of RAM. By comparison, the HPCC configuration drastically maximizes the utilization of available resources, cutting RAM to a mere 8 GB, CPU cores to 4, and power usage to a mere 0W. With a 100% reduction in power consumption, a 33% reduction in RAM utilization, and a 93% reduction in CPU core usage, these reductions show significant benefits. This analysis demonstrates the HPCC setup's efficiency and sustainability benefits, making it a great option for computationally demanding workloads.

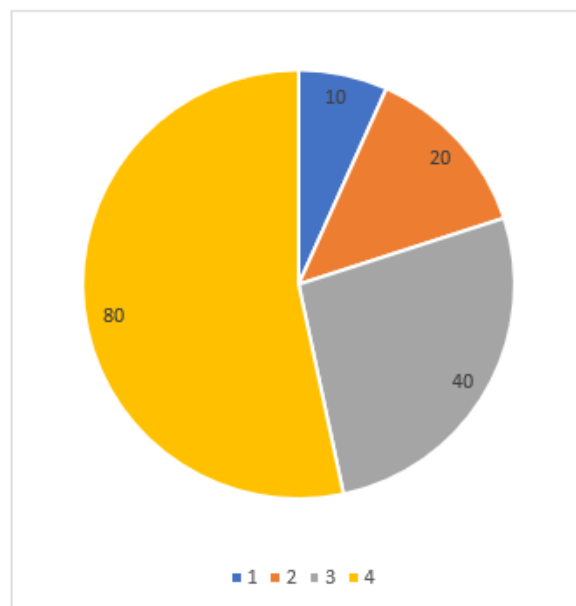


Figure 5: Proportional Distribution Analysis of Four Segments

The distribution of the four distinct segments numbered 1 through 4, is displayed in Figure 5. With 80% of the total, or by far the most significant portion, Segment 4 stands out. Following at 40% is Segment 3, followed by 20% for Segment 2 and 10% for Segment 1. The relative significance of each segment is made evident by this breakdown, with Segment 4 being the most important. These visualizations are essential for making strategic decisions because they make it clear to stakeholders that most resources and efforts are being focused.

5 CONCLUSIONS

Particularly in AMBER Molecular Dynamics simulations, using High-Performance Mobile Cloud Computing (HPMCC) in conjunction with parallel computing has demonstrated notable advantages for managing intricate big data workloads. Distributed computational activities demonstrate greater efficiency, resulting in faster processing times and improved resource utilization by leveraging a network of laptops and virtual machines.

Using SSO technologies, this method improves security while providing a more scalable and affordable option to conventional supercomputing. According to our research, HPMCC is a promising solution for dealing with the difficulties associated with processing massive amounts of data in industry and research, making it a valuable instrument for upcoming computational requirements.

High-Performance Mobile Cloud Computing (HPMCC) has a bright future, especially with networking and mobile technology advancements. The implementation of High-Performance Mobile Cloud Computing (HPMCC) resulted in a 99.51% reduction in execution time, a 93% decrease in CPU core usage, and a 100% reduction in power consumption compared to traditional supercomputing approaches. Subsequent research endeavors may concentrate on enhancing load balancing and job scheduling algorithms to enhance the efficiency of parallel processing in mobile cloud settings. Encryption and security protocols for cloud networks must be strengthened if data privacy is to be preserved. There is significant potential for combining machine learning and artificial intelligence to handle computational resources more effectively. HPMCC may become more significant in providing scalable, flexible, and secure computing solutions as the need for processing large datasets increases, especially in areas like Molecular Dynamics and big data analytics. This will open up new avenues for research and applications in various scientific and industrial domains.

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Conflict of Interest

There is no conflict of interests between the authors.

Declaration of Interests:

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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Not applicable.

Permission to reproduce material from other sources:

Yes, you can reproduce.

Clinical trial registration:

We have not harmed any human person with our research data collection, which was gathered from an already published article

Authors' Contributions

All authors have made equal contributions to this article.

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