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Accelerating Scientific Discovery Through High Performance Computing: Challenges and Opportunities for Africa Researchers

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Abstract

High Performance Computing (HPC) has the potential to accelerate scientific discovery in Africa, but the continent faces several challenges that must be addressed to fully realize its potential. These challenges include limited access to HPC resources, limited technical expertise, limited data infrastructure, and funding constraints. However, there are also significant opportunities in accelerating scientific discovery through HPC in Africa, including collaborative research, enhanced research capabilities, improved data management, improved public health, production engineering and capacity building. By addressing these challenges and fully leveraging the power of HPC, African scientists can make important contributions to global scientific knowledge and innovation, driving further development in the continent and beyond.

Keywords

High performance Computing, cloud computing, challenges, Opportunities, Research groups, collaboration, Engineering

Introduction

High-Performance Computing (HPC) refers to the use of advanced computing systems to solve complex scientific, engineering, and data-intensive problems. HPC has revolutionized research and development in various fields, including weather forecasting, drug discovery, genomics, and more. According to (Daniel R., 2022) High Performance Computing (HPC) has relative influence of governments and traditional computing companies on the scientific computing ecosystem has waned, with important implications for science and engineering discovery via leading edge high-performance computing (aka HPC or supercomputing). It is also a field of computing that focuses on the development of advanced hardware, software, and algorithms to enable the processing of massive amounts of data at high speeds. High-performance computing has become an essential tool for accelerating scientific discovery by enabling researchers and scientists to solve complex computational problems that would be impossible to tackle using traditional computing methods. HPC systems have been used to simulate complex systems, analyze large datasets, and conduct advanced mathematical calculations that have led to breakthroughs in a wide range of fields. Cloud computing is likely to benefit and support science and engineering applications, data mining, IoT, computer finance, Production Engineering , gaming, and social networking, as well as many other high-performance computing and data-intensive activities (Vingi. P. N et al. 2022). Moreover, in various fields, Offering an HPC service could tailored for relevant advantages that go beyond the possibility of analyzing massive amounts of data in a timely manner. With this knowledge, it introduced researchers to the HPC work environment, raising their awareness of the opportunities offered by HPC and thus making more likely the future development of tools, algorithms, applications and implementations optimized for HPC environments possibly stemming a positive feedback loop (Tiziana C., etal, 2020). High performance computing availability is thus becoming a key factor in making effective use of high throughput sequencing (HTS) data, that is extracting meaningful information in a (Goodwin S, 2016) reasonable amount of time.

The paper discusses challenges faced by HPC in Africa which including infrastructure limitations, scalability, and the need for advancements in hardware technologies. The research work highlights the significance of HPC in Africa and the opportunities it presents for innovation, collaboration, and development. By addressing challenges and leveraging the power of HPC, African scientists can contribute to global scientific knowledge and innovation. It also present the importance of HPC in enabling African researchers to process large amounts of data quickly, collaborate globally, and contribute to addressing critical challenges such as climate change, public health, and food security. Then give African institutions and facilities that has such initiatives; such as the African School on Electronic Structure Methods and Applications (ASESMA), CApic-Ace, KENET and regional HPC centers that aim to develop expertise and infrastructure in Africa.

Literature Reviews

In supercomputer, all of its power is utilized to execute few programs as efficient as possible. Scientific and engineering applications require large number of computations; to do so, we need additional processors, shared memory, and multiple disks. Supercomputers are transistorized to handle large numbers of computations. They are capable to process huge amount of calculations for complex jobs while HPC makes use of supercomputer and computer cluster technologies, it applications are mainly categorized into two types; which they are closely coupled applications and loosely coupled applications (John S. P, 2011). To run these HPC applications it requires costly hardware, and users have to wait to make use of the shared memory. With the advent of Cloud Computing and benefits of Infrastructure as a service (IaaS) and Platform as a service (PaaS), scientists and engineers are able to deploy their HPC applications in the cloud without worrying about the costs associated with infrastructure and other costs (Sindhu, 2012). Moreover, are different applications which are running in cloud like Molecular modeling, Genome analysis, oil, Gas, Computer science, Product Engineers etc. Cloud computing is captivating to scientists in the small research groups in fields of computational science and engineering.

By using Cloud Computing, research groups could perform high performance calculations by these HPC applications. The cost for running that application should be known to vendors by analysing the cost of deploying the infrastructure at a region. Research groups or vendors can also know the return of investment and cost estimation can which can be determine by which applications can use cloud. They should know whether to run a part of application or complete application in Cloud to save money and resources i.e. in terms of cost, performance and infrastructure. More also, (Truong H. L and Dustdar, 2010) scientists should use their known performance characteristics (e.g., transferred data, execution time) of their applications to analyze and estimate cost. Some of the cost models are provided by cloud providers in their pricing specification. Basic cost models that are provided by cloud providers in pricing specification are Mds (Data storage), Mcm (Computational machine), Mdfi (Data transfer into the cloud), and Mdfo (Data transfer out of the cloud).

In recent years, there has been a growing interest in bringing HPC to Africa, as many African countries are seeking to develop their scientific and technological capabilities which enable researchers and scientists in Africa to process large amounts of data quickly and efficiently, and to collaborate with colleagues around the world. HPC in Africa will post some significant opportunities to drive innovation, collaboration, and development in the region. By addressing some challenges and fully leveraging the power of HPC, African scientists can make important contributions to global scientific knowledge and innovation.

In Africa, HPC is becoming increasingly important in advancing research and development. HPC can enable African researchers to simulate and model complex systems, analyze large datasets, and run advanced algorithms that were previously not possible. This can lead to breakthroughs in fields such as agriculture, healthcare, energy, in a wide range of scientific and engineering applications, including climate modeling, drug discovery, aerospace simulations, and many more.

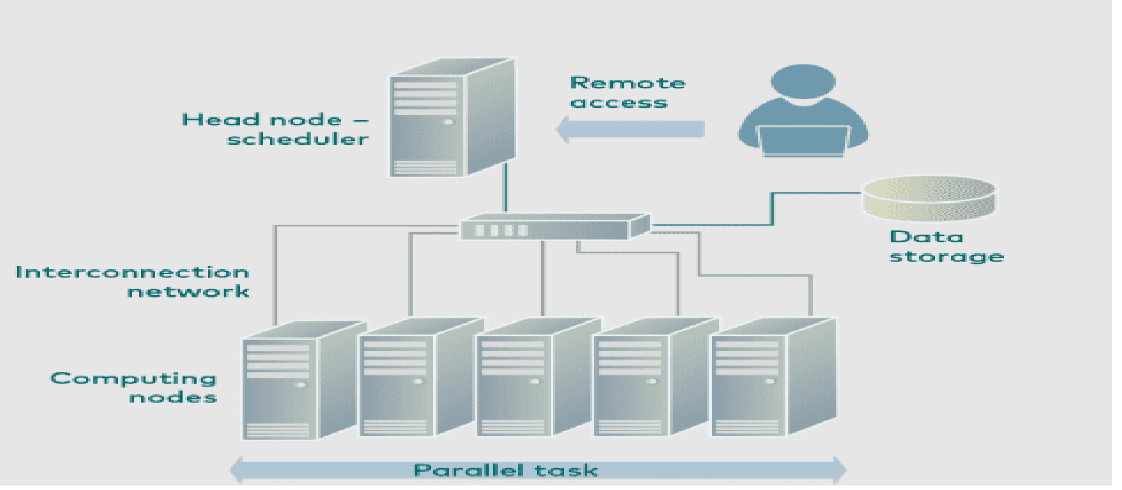

Figure 1: HPC Cluster Architecture

Adapted from https://cloudinfrastructureservices.co.uk/what-is-hpc-high-performance-computing-and-how-it-works/

Recently, African nations are increasingly embracing High Performance Computing (HPC) to enhance their technical and scientific capabilities, enabling efficient data processing, simulation, and execution of advanced algorithms, and promoting research and development (Amolo G., 2018). HPC technology could lead to innovations in energy, healthcare, and agriculture industries. More-likely, It is widely used in various technologies such as IoT (internet of things), Artificial intelligence, and 3D evolutional images solving complex problems. All these applications uses a large amount of data exponentially. HPC is a fast computing application, so we can use it parallel with CPU and GPU. More also, HPC has revolutionized research in fields like weather forecasting, drug discovery, genomics, and physics, enabling breakthroughs in various fields by simulating complex systems and analyzing vast data.

S/N	**HPC FACILITIES IN AFRICA**		
	SERVER MODEL	**BRANDS**	**COUNTRIES**
1	AMD Operon-based IBM e150 (Has eight nodes equipped with clear speed accelerator card)	IBM	South Africa
2	IBM Blue Gene/Prack	IBM	South Africa
3	Hybrid SunMachine (SPARC 64 VII M700)		South Africa
4	4 Computing Nodes 2.5 Teraflops, Linux, Redhat OS	Brand Unknow	Tanzania
5	Dell PowerEdge 2950 Headnode and 1950 computer node	DELL	Nigeria
6	Four (4) Computer Nodes	Brand Unknow	Nigeria

Some few Africa Countries are Ghana, Malawi, Senegal, Cameroon and so on.

Table 1: African Countries that has HPC in recent years

Regional initiatives in Africa have established small HPC facilities for local researchers and graduate students, with support from the Chinese government. In Kenya, the Kenyan Education Network is assisting a special interest group, Computational Modeling and Materials Science, by offering workshops on HPC resource usage and proposal writing (KENET, 2023). The African School on Electronic Structure Methods and Applications (ASESMA) introduces computational modeling to African academia, researchers, and graduate students, with biannual series planned from 2010 until 2020 (Chetty N., etal, 2010). The 2010 series was held in Cape Town, with those in 2012, 2015 and 2016 taking place in Eldoret (Kenya), Johannesburg (South Africa), and Accra (Ghana), respectively. (Amolo G., and Martin R. H, 2015) The initial focus was on materials science, with physics and chemistry as the fundamental subjects, but has grown to involve biological systems and applied sciences such as materials engineering. The CHPC now has a much larger user base that includes drug design and astronomy, among others. More also, CApIC-ACE in Nigeria aims to develop indigenous African scientists with bioinformatics, molecular biology, and engineering skills for research in malaria, prostate, breast cancer, and personalized medicine. Collaborating with institutions in Nigeria, West Africa, Germany, France, US, and UK. (CApIC-ACE, 2023).

Challenges of HPC in relation to Africa:

In Africa, there are several challenges that researchers in Africa face when it comes to HPC adoption, this research will discuss on these challenges.

There are some significant challenges to overcome when it comes to accelerating scientific discovery through HPC. One of the main challenges is scalability. As HPC systems become larger and more complex, it becomes increasingly difficult to manage and coordinate the resources needed to execute computations efficiently. This has led to the development of new approaches to programming and optimizing HPC systems, including the use of machine learning and artificial intelligence techniques. According to (Tiziana C., etal, 2020) having a good mix of general-purpose computational power, the possibility of booking an arbitrary number of cores (multi-threading) or nodes for the jobs that require more CPUs, or very large memory nodes for jobs with large memory requirement, has been shown to be a very efficient and affordable infrastructure for data analysis. Without expertise on system design and performance tuning, libraries that provide generic APIs for coupling scientific workflows in various application can significantly impact the workflow performance and scalability (Dan etal, 2022) .

Another challenge is the need for specialized hardware and software that can handle the unique requirements of scientific computing. This includes the development of specialized processors, memory systems, and networking technologies that can provide the high bandwidth and low latency required for scientific applications. It's becoming more and more common that the hardware requirements needed to perform a convenient frame of time far exceed those available in desktop computers, servers, and even local Information Technology (IT) facilities **(**Tiziana C., et al., 2020**)**. HPC systems are rapidly evolving with new architectures and hardware, and in some cases the hardware interfaces are proprietary, such as the Cray interconnect (Dan H., etal 2022).

Infrastructure (Limited access to HPC resources): One of the biggest challenges facing African scientists is limited access to HPC resources, (Dan R., 2022) market and cost pressures have driven most users and centers away from specialized, highly integrated supercomputers toward clustered systems built using commodity components. In cases where such facilities exist, the cost of maintenance is prohibitive, leading to long periods of inactivity due to lack of spare parts, and eventually abandonment in many cases (Amolo G., 2018). HPC requires a robust data infrastructure to support large-scale simulations and data processing. Typically, the computationally intensive parts of the application are offloaded to the GPU, which serves as the CPU's parallel co-processor. Today's modern supercomputer systems, in practice, consist of many nodes, each holding between 2 and 32 conventional CPUs and 1–6 GPUs. There will usually also be a high-speed network and a system for data storage. Many African countries lack the necessary data infrastructure to support HPC (Dan R., 2022).

Funding constraints: Developing and maintaining HPC systems can be expensive, and many African countries face funding constraints that limit their ability to invest in HPC. Without Government investments and making modalities and ideas from designing and funding of supercomputers which could be shaping the next generation of mainstream and consumer computing products that would assist researcher to be less dependent on foreign nation. Funding HPC would potentially serve as a sandbox for computational and research software developers to build their own open tools, conduct small-scale user testing and gather feedback for relevant output at our environment.

Limited technical expertise: Developing and maintaining HPC systems requires a high level of technical expertise, which is often in short supply in Africa. This can make it difficult for African scientists to take full advantage of the power of HPC. Inefficient management of resources has a clear and direct significant negative influence on efficiency and cost, and an implicit impact on the system operations. Due to poor efficiency, certain functions can become extremely costly or even ignored (Vingi. P. N et al. 2022).

Others include Ecosystem factor (cooling system), political factor, policy. However, there are initiatives aimed at addressing these challenges, including the development of regional HPC centers such as the African Research and Education Network (AfREN) and the training of African researchers in HPC techniques, and collaborations between African and international institutions.

Opportunities of HPC in relation to Africa:

Despite these challenges, there are also significant opportunities for accelerating scientific discovery through HPC. For example, HPC can be used to simulate the behavior of complex systems, such as weather patterns or biological processes, providing insights that would be difficult or impossible to obtain through experiments alone. HPC can also be used to analyze large datasets, such as genomic data or climate data, to uncover patterns and correlations that can lead to new discoveries.

Collaborative research: HPC can enable African scientists to collaborate with colleagues around the world on complex research projects. Access to HPC resources to support strategic and focused experimental research might be key to Africa's growth in an effort to diversify revenue generation (Amolo G., 2018) and can lead to the exchange of ideas and expertise, and can help to drive scientific and technological development in Africa.

Enhanced research capabilities: By providing access to powerful computing resources such as (Daniel R., 2022) graphics processing units (GPUs), predominantly developed by NVidia, have emerged as a powerful platform for high-performance computation and have been successfully used to accelerate many scientific workloads and to support both computer gaming and AI. HPC can enable African scientists to conduct more complex simulations, modelling studies, and data analysis, leading to new discoveries and breakthroughs.

Improved data management: HPC can help African scientists to manage and analyze large datasets more effectively, enabling them to draw insights and make more informed decisions. Data security imposes a significant importance in this Computation. Data need to be vulnerable for unknown users to access.

Improved public health: HPC can be used to develop advanced models for predicting disease outbreaks and tracking the spread of infectious diseases. This can help public health officials to respond more quickly and effectively to outbreaks, saving countless lives in the process.

Capacity building: By investing in HPC infrastructure and expertise, (Daniel R., 2022) designing and constructing leading edge high-performance computing systems must change in deep and fundamental ways, embracing end-to-end co-design; custom hardware configurations and packaging; large-scale prototyping, and collaborative partnerships with the dominant computing ecosystem companies. Now a days, HPC in Cloud came into existence to solve some of the technical and enterprise problems where (Karthik P. and Sumanth M., 2012) African countries can build capacity and enhance their scientific and technological capabilities, attracting and retaining top talent and driving further development.

Development in the region: government investments and the insights and ideas from designing and deploying supercomputers shaped the next generation of mainstream and consumer computing products (Daniel R., 2022). the introduction of HPC to Africa has the potential to transform scientific and engineering research on the continent, and to help address some of the most pressing challenges facing society today.

Conclusion:

There are several challenges facing the acceleration of scientific discovery through HPC in Africa, while there are also significant opportunities to drive innovation, collaboration, and development in the region. These challenges and opportunities of HPC for scientific discovery are closely intertwined. As researchers and scientists continue to push the boundaries of what is possible with HPC, new challenges will emerge, but so too will new opportunities for accelerating scientific discovery and making breakthroughs in a wide range of fields. African scientists can make important contributions to global scientific knowledge and innovation. If you are a researcher in Africa interested in HPC, there are several steps you can take to get started. First, familiarize yourself with the basic concepts and technologies behind HPC. This can involve taking courses, attending workshops or conferences, and networking with experts.

Another important consideration in the introduction of HPC to Africa is the need to ensure that this technology is used to address the most pressing challenges facing the continent, such as climate change, public health, data security and food security. By harnessing the power of HPC, African researchers can contribute to global efforts to tackle these and other critical issues.

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