A BRIEF CENTRE OFAPPLIED MATHEMATICS & SIMULATION ADVANCED RESEARCH CENTRE (AMSARC)

AMSARC, a research Centre whose interests span Physical sciences, Applied Sciences, Engineering, and Technology is one of SHESTCO's autonomous interdisciplinary research Centre. The Centre which was until July 2019 an appendage of Physics Advanced Research Centre (PARC) is mandated to advance research in applied mathematical sciences, train research manpower, develop and maintain advanced mathematical and scientific computing foundations to accelerate the pace of scientific discoveries in SHESTCO. AMSARC's R&D activities though complementary, differs from those of other Centres by serving majorly as an arena or a melting point where mathematical theories, concepts, methodologies and algorithms as well as computational modelling and simulations collide with experimental observations and measurements. Being the epicentre of contemporary R&D innovations

AMSARC is also charged with the responsibility of developing, designing and managing internationally accessible research database system for innovative and dynamic R&D activities in SHESTCO.

Currently, the centre is compartmentalized to function in three (3) outstanding inter-disciplinary units namely Computational Modelling/Simulation and Optimization engineering, Automated Learning Frontier & Artificial Intelligence Engineering and Research Database Management and Software Performance Engineering.

i. Computational Modelling/Simulation and Optimization Engineering

(i) To research and develop scalable mathematical models, theories, algorithms, and their implementations to address rigorous scientific and engineering challenges,

(ii) To develop scalable numerical methods encapsulated in robust Mathematical and statistical computational software libraries that enable scientific analysis and simulation on high performance computer (HPC) systems.

(iii) To research, develop and provide structured manpower training, facilities, workshops, conferences, seminars and symposiums on innovative computational methods, modelling and simulations, as well as their related software utilization to Nigerian R&D environment.

ii. Automated Learning Frontier & Artificial Intelligence Engineering

(i) To research and develop fundamental aspects of computer vision, machine learning and data analytics for artificial intelligence (AI) applications, imaging recognition, object detection as applied to disease prediction and other important aspects.

(ii) To research and develop robust analytical and numerical methods and algorithms as well as tools as portable high-performance software applications for computational analysis, modelling and simulation.

(iii) To research, explore and utilize the principles of supervised and unsupervised learning frontiers toward providing robust foundations for Machine Learning, data analytics and Artificial Intelligence applications in the Nigerian R&D environment.

(iv) To research, develop and provide structured manpower training, facilities, workshops, conferences, seminars and symposiums on advanced Machine Learning, data analytics and Artificial Intelligence applications, as well as their related software applications to Nigerian R&D environment.

iii. Research Database Management & Software Performance Engineering

(i) To research, develop and manage bits and bytes of research data/information for optimal scientific insights; thereby providing efficient and reliable techniques/tools for storing, transferring, accessing, and manipulating extremely large data. The goal of which is to enable researchers to analyse, visualize and query these large datasets for new scientific discoveries and breakthroughs.

(ii) To research and develop innovative approaches to scientific software utilization for system performance analysis, as well as for model simulation and optimization.

(iii) To research, develop and maintain internationally accessible computing foundations, with communications and research database management systems for innovative and dynamic R&D activities.

(iv) To serve as a Centre for the dissemination of scientific research datasets, information and publications for public consumption.

(v) To serve as a numerical backbone for scientific productivity through the developmental design and to serve as custodians of advanced computational software infrastructure for scientific computing and analysis.

(vi) To research, develop and provide structured manpower training, facilities, workshops, conferences, seminars and symposiums on research database utilization and management, computing device applications, as well as their related software utilizations in Nigerian R&D Environment.

Computational Software Performance Engineering for Advanced Multi-scale Modelling and Simulation.

The journey towards finding a sustainable solution to the myriad of socio-political and economic problems confronting Nigeria, and insecurity in particular, tends to defy known qualitative case study analyses of the social science discipline, hence, proliferation of diverse institutions of organized crimes in recent times. Novel mathematical modelling, computational analysis and numerical simulations driven by innovative scientific software libraries are fast becoming the essential elements of all aspects of any nation's R&D activities.

The multiplicity of the cross-disciplinary nature of contemporary computational sciences has underpinned such beneficial modern capabilities like Internet of things (IoT), Machine Learning/Artificial Intelligence (AI), Cyber Security, Medical image processing, Computer animation, Numerical weather predictions, and all types of digital communications. Novel computational software-driven capabilities, allow researchers to combine the rich detail of qualitative case study analysis with the rigor of voluminous data-oriented quantitative analyses, and computational research at high speed and precision, as well as the virtual visualization of complex structures and processes within the boundaries of a theoretical model.

Advancement in multi-scale modelling/simulation techniques employ mathematical computational software libraries, to quantitatively represent, describe and numerically simulate a system at more than one scale, while functionally linking the models across different scales. This inter-play of innovative mathematical software-driven computational sciences and multi-scale analysis can be viewed as the "third paradigm" of scientific discovery, alongside theory and laboratory experiments.

The development, sustenance and growth of innovative computational software libraries which run on AMSARC's modest cluster of High-Performance Computers (HPC), are required for the analysis/simulations of a vast range of complex physical, socio-economic and engineering systems such as insurgency, internet fraud, disease epidemiology, Energy and Agro-economy, political conflicts and salient other physical and engineering problems. This allows for understanding and management of these systems at high level of precision.

Contemporary researchers, and indeed, the nation's socio-economy and security stakeholders, therefore, require AMSARC's state-of-the-art approach and facilities to gain new scientific insights, for a sustainable R&D and technological development. Therefore, if SHESTCO's R&D facilities must keep pace with the contemporary scientific, technological and innovative drives of applied mathematics, computer science and data analytics; which are essential enablers of contemporary computational sciences, the autonomy, development, sustenance and growth of AMSARC must be the basis for its insights and discoveries.

Research Work Carried out in AMSARC:

It's worth mentioning that over the recent years, AMSARC in collaboration with other SHESTCO's Centres has deployed the novel computational software-driven applied mathematical modelling and simulation

approaches to develop prototype models for studying the performance measures, as well as synergizing the ultimate solutions of key socio-political, economy and physical systems. Key research exploits in its archives includes:

(i) The Boomerang Effect of Some Counterterrorism (CT) Measure: A Mathematical Perspective published in six international languages)
(ii) The Counter-terrorism Resource Allocation Queuing Fairness Appraisal of Leadership Decapitation Approach.
(iii) Resources Allocation Queue-Fairness Model of A Multi-Server Priority System of Petroleum products Distribution System in Nigeria.
(iv) Optimizing Community's Supports for effective Counter-terrorism Operations: A Sticks-Carrots Game Theoretic Model.
(v) Optimal Human Resources Allocation in Counter-Terrorism (CT) Operations: A Mathematical Deterministic Model.
(vi) Assessing the Effectiveness of "Carrots and Sticks" Approach on Terrorists' Strength and Sustainability: A Mathematical Deterministic Model.
(vii) Understanding the Condition under which Decapitation Strategy Can Impact on Terrorists' Strength and Sustainability: A Mathematical Perspective.
(viii) Understanding the Implication of Some Counter-Terrorism (CT) Measures: A Mathematical Perspective.
(ix) The Systemic Approach to Combating Terrorist Organization: A Mathematical Conceptualization
(x) Design of a Data Acquisition and Logging System for Air Quality Monitoring and Meteorology Applications.
(xi) Electrochemical Investigation of the Effect of Activated Coconut Shells in the Negative Plate of Lead Carbon Battery.
(xii) A Comparative Study of Physicochemical, Proximate and Minerals Analysis of some Underutilized Wild Edible Seeds used as Condiments in Nigerian Traditional Soups.
(xiii) Comparative Study of Chronic Kidney Disease Predictor Performance Given Insufficient Training Dataset. Information Technology and Management Science.
(xiv) A Constrained Proper Orthogonal Decomposition Model for Upscaling Permeability.
(xv) An Anonymous IoT-Based E-Health Monitoring System Using Blockchain Technology.
(xvi) Numerical solutions of covid-19 SIRD model in Nigeria.
(xvii) The Solution of a Mathematical Model for Covid-19 Transmission and Vaccination in Nigeria by using a Differential Transformation Method.
(xviii) Approximate Solutions of Malaria Disease Transmission Model: Using Multi-Step Differential Transform Method.
(xix) The performance measure of a state dependent terror queuing model: A comparative assessment of counter-terrorism (CT) options.
(xx) A Structural Equation Model of Security Workforce Performance and Strategic Job Requirements: The Nigerian Security and Civil Defence Corps Perspective.
(xxi) The Syndromnization of Intelligence Measures in Counter-Insurgency Environment: A Mathematical Conceptualization

Deployment of High Performance/Parallel Computing (HPC) System to SHESTCO R&D Activities

The incursion of Information Communication Technology (ICT) into R&D activities has revolutionized the stress/risk oriented and mechanistic procedures of accessing, processing and analysing data; by engaging a network of powerful computer systems and parallel computing techniques to solve advanced and complex computational problems.

With innovative scientific software libraries run on AMSARC's HPC system, large volume of data and information from network of workstations PCs can be coordinated, correlated, processed, analysed and simulated centrally for on-the-spot results and rapid decision making. This deployment of AMSARC's HPC

system for advanced R&D activities, enables wearisome and risk-oriented mechanical, chemical and biological experiments as well as fragile technological processes to be coordinated, simulated and visualized centrally from a network of workstations PCs and the results displayed on integrated High-Definition Visual Display Units (HD-VDU) for rapid decision making.

Other key contemporary scientific and technological innovations, applications, benefits and contributions of AMSARC's research facilities to SHESTCO R&D community include:

(i) Machine Learning/Artificial Intelligence (AI) modelling for predictive analysis,
(ii) Molecular Dynamics: computation, molecular simulation and visualization of research results,
(iii) Structured training and capacity development on advanced computational researches and utilization of its related scientific software infrastructures, and
(iv) Acquisition, custody and deployment of advanced computational software infrastructures to SHESTCO R&D activities.

Machine Learning/Artificial Intelligence (AI) Modelling:

Since time immemorial, statistical methods have been used to perform data processing, analysis and projections. In recent times, these classical statistical methods have not quite been flexible enough in identifying new variables as well as incorporating creative changes in the experimental observations. However, owing to the improvements in the performance of computational software libraries in recent times, as well as active development by various software contributors, Machine Learning/Artificial Intelligence has become a favourite choice in modern statistical research.

AMSARC employed Machine Learning/Artificial Intelligence algorithms to create mathematical models which utilize sample data to make predictions or take decisions without being explicitly programmed to do so. Machine Learning/Artificial Intelligence algorithms can be utilized in pattern recognition, facial recognition and object recognition with tracking in surveillance systems. For instance, in Collaboration with AMSARC, an implementation of object recognition with tracking was carried out at the PARC in her initial solar-thermal generator's prototype design in order to track the sun.

Machine Learning/Artificial Intelligence algorithms find versatile applications in virtual screening methods in drug discovery. Machine learning/Deep learning algorithms are trained with a vast set of available data to prioritize a collection of molecules as an active agent against a particular protein target, thereby identifying potential drug candidates while saving time and cost. This helps to rapidly shorten the drug-lead discovery path.

Molecular Dynamics, Computation, Molecular Simulation & Visualization:

In contemporary investigation researches, prediction or optimization of properties of a material, computational modelling technique such as ab-initio electronics structure and molecular dynamics calculations with visualization, can enable researchers to gain insight into the atomic-level dynamics of the material. These can be employed in the design and development of resilient, efficient, low-cost and sustainable revolutionary materials. Indeed, a variation of these methods can be used to understand the complexity of the structural dynamics in biomolecules.

Also, with AMSARC's computer-aided drug design capabilities, it is possible to simulate and predict whether a given molecule will bind to a target as well as estimate the strength of the affinity. These and many more computational methods have been used by successful scientists and pharmaceutical companies over the years in improving biological systems. Hence, the availability of this innovation, knowledge and skillsets in AMSARC is a major contribution to R&D activities in SHESTCO.

One of AMSARC's contributions is enhancing the discovery of novel and better medicines using computational methods. AMSARC seeks to engage in the utilization of existing algorithms as well as developing new ones to accelerate the simulation of pharmaceutical processes and biological relevance, such as the interaction of proteins and potential drug candidates or the prediction of biological structures. This can be implemented on multicore central processing unit (CPU) enterprise servers in an internal cluster or on mixed CPU-GPU architectures. Though, AMSARC is not currently equipped with GPU hardware, however, it is noteworthy to mention that since computer simulations are generally computationally intensive, it would

be more practical to take advantage of the speed-up provided by GPU-accelerators in our HPC system which executes programs that implement parallel processing, thereby producing high throughput.

Structured Training, Skill Acquisition and Capacity Development:

The enhancement of researchers' capacity and the acquisition of versatile technical skills are key parameters in expanding problem-solving capabilities on the beneficiaries. AMSARC particularly achieved this noble feat through teaching young or inexperienced scientists, and equipping undergraduate and graduate students with computational research skills; training and retraining of personnel and executing multi-disciplinary collaboration through conferences, workshop and webinars. AMSARC maintains active visitors' program for SIWESS students, graduate internships, and academics, as well as organizes international conferences, workshops, webinars and symposium in Applied Mathematics and its applications.

AMSARC's fledgling advanced computing research, employed virtual class room system to disseminate knowledge and skillsets in the areas of advanced computational studies, providing a central hub where researchers can access and utilize high performance computational software resources, Mathematical modelling, analysis, and programming skills. This enables upcoming research scientists to develop their computing career as well as receiving support in various areas of research interest. Through these and other inclusive computational education programs, AMSARC can support individual career development and strengthen institutions in areas of (i) computational discovery and designs, including receptor-ligand interaction prediction, molecular dynamics computations, and molecular docking (ii) computational material science studies (iii) computational fluid mechanics, and (iv.) computational modelling, simulations and optimization of physical systems.

It's also worth mentioning that in the recent past, AMSARC, in collaboration with research-related industries, other SHESTCO's Centres, and governmental bodies had organized and hosted a number of training workshops, conferences and webinars in some of the above-mentioned areas. Significantly,

- In September 2021, AMSARC, in collaboration with a scientific Software vendor – Tangier International Company Limited, had organized and hosted a 4-day international training workshop on *"Modelling and Simulation Solutions using Maplesoft and Maplesim Software"*. The workshop which drew both physical and virtual participants from academia, research institutions and industries helped to foster synergy for knowledge-base integration and applications of innovative computational software infrastructure – Maplesoft and Maplesim, in the Nigerian R&D community.
- In November 2023, AMSARC also collaborated with Biotechnology Advanced Research Centre (BARC), to host a 5-day international training workshop on *"Bio-informatics Skills Acquisition for Researchers and professionals"*. The workshop also drew physical participants from academia and research institutions in Nigeria, and hitherto help to foster synergy for knowledge-base integration and applications of computational modelling/simulation in biotechnological researches in Nigerian R&D institutions
- Also in December 2023, AMSARC, in collaboration with Federal Ministry of Science, Technology and Innovation had organized and hosted a 5-day national training workshop on *"Basic Computer Skill Acquisition for vocational technical teachers*" drawn from selected technical colleges in Nigeria. The workshop, was not only aimed at fostering synergy for knowledge-base integration and applications of computational knowledge but also equipped participants with basic computer skills and capabilities required to function effectively as contemporary teachers in Nigerian vocational and technical colleges.

Acquisition, Custodians and Deployment of Advanced Computational Software Infrastructures:

As observed earlier, computational modelling, analysis, and simulations driven by innovative scientific software infrastructures are fast becoming the essential elements of contemporary R&D activities. A central hub where researchers, students and professionals can embark on independent or collaborated computational research, analysis, modelling and simulation of complex real-world systems using versatile software infrastructures, as well as acquiring the necessary expertise and skillset as has been AMSARC's major preoccupation since her inception in 2019. The acquisition, custody and deployment of some versatile computational software libraries run on AMSARC's HPC have been the Centre's major breakthrough over the

recent years. At present AMSARC's central HPC server is deployed, harbours and runs the following key proprietary and open-source software libraries to support and stimulate R&D activities in SHESTCO:

- MATLAB Software (MLSMS)
- MATLAB SIMULINK (SLSMS)
- MATLAB Partial Differential Equation Toolbox (PDSMS)
- MATLAB Statistics and Machine Learning Toolbox (STSMS)
- MATLAB Symbolic Math Toolbox (SMSMS)
- Maplesoft and Maple SIM
- Python (Anaconda) suite
- R & R-Studio suite

Its worthy of note that these software libraries have contributed immensely to AMSARC's major breakthrough in her current R&D activities.

CURRENT RESEARCH PROJECTS IN AMSARC

Considering the level of socio-political, economic and security challenges bedevilling the Nigerian state in recent times, AMSARC's research lens has been categorically tilted toward the following key and inter-disciplinary research areas:

(i) Leveraging artificial intelligence and machine learning techniques for enhanced effectiveness and efficiency of scientific research and development activities.

(ii) Deployment of Advanced Computational and Multi-Scale Modelling/simulation and Optimization foundation on Health Care management, Agricultural and Security studies in Nigeria.

(iii) Deployment of Advanced Machine Learning & Artificial Intelligence (AI) Based Modelling/Simulation foundation on Health Care management, Agricultural and Security Studies in Nigeria.

(iv) Deployment of Advanced Information Management System and innovative computational Software utilization foundation for Nigerian R&D environment.

As a developing nation, Nigeria cannot afford to be left behind with moribund R&D approaches by contemporaries if sustainable scientific discoveries must be made. Therefore, the government should act as a catalyst to support, domesticate and grow this novel initiative by upgrading AMSARC to its full independent potential, fund the growth of Advanced Mathematical Computational software development in her R&D institutions. To widen the scope of technology applications in Nigeria R&D institution, AMSARC is a veritable tool in the wheel of progress in the nation's technological evolution. A wholesome partnership, collaboration and patronage by the private sectors and other government agencies should be encouraged so as to widen the scope of utilization of this novel scientific idea for more result-oriented R&D activities.