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Review article

Advances in Nanoscience and Nanotechnology

Computational Nano-Science and Nano-Technology

Aderemi Kuku

National Mathematical Centre, Abuja, Nigeria

***Corresponding author**
Aderemi Kuku, Distinguished Professor of Mathematics, National Mathematical Centre, Abuja, Nigeria. E-mail: aderemikuku@yahoo.com

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Abstract

This article, which is concerned with computational Nanoscience and Nanotechnology (CN&N) at first, presents an overview of CN&N from historical perspective, benefits and concerns. It then discusses the place of mathematics vis-à-vis other areas of science and technology (including CN&N), and then presents numerous technologies (including nano-technology) that would not exist today without mathematics. Finally we exhibit some mathematical techniques used in CN&N and briefly points the way forward.

Introduction

In this paper, we present Computational Nano-Science and Nano-Technology as multidisciplinary fields that encompass the four areas of Science and Technology-Basic sciences, Applied Sciences, Classical and High Technologies---which we view as concentric layers with diffuse boundaries with a central core of basic sciences and mathematics at its innermost core such that theories from the inner cores of basic sciences and mathematics help to solve problems in applied science and technology while problems arising from the outer layers of applied sciences and technology provide the inner cores of basic sciences and mathematics with new structures, new concepts and new methods. It is clear from the examples given in the paper that the growth of Nanoscience and Nanotechnology has followed the pattern outlined above.

At first, we present in section 1 an overview of Nanoscience and Nanotechnology-with some historical perspective, as well as some benefits and concerns associated with the subject. In section 2, we present the nature and structure of mathematics relative to the four areas of science and technology in some details emphasizing the interconnectedness between them through the concentric layer philosophy outlined above, We then discuss the role of ICT. In section 3, we provide numerous examples of technologies (including nanotechnology) that would not exist today without mathematics as well as provide in section 4 specific examples of mathematical techniques used in computation Nanoscience and nanotechnology.

In section 5, we provide a brief way forward for this exciting relatively new subject

Section one
An Overview of Computational Nanoscience and Nanotechnology

Some Generalities on Nanoscience and Nanotechnology

The goals of Materials Science and Materials Technology (of which Nanoscience and Nanotechnology constitute a part) include understanding, studying, synthesizing, and maximizing the use of existing materials as well as create new ones. Such materials include polymers (including biological polymers); composites (heterogeneous materials made up of two or more materials); metals; ceramics; rubber; textiles and fiber materials; electrical, optical and magnetic materials; biological materials used for tissue design and engineering for health care purposes; nanomaterials, glass processing; electro chemicals; fine chemicals, etc, etc.

Nanoscience is the study and control of the finest of particles on the nanometer scale (one nanometer is one billionth of a meter-in fact nano refers to one billionth of a unit of measurement) while Nanotechnology is the application of nanoscience leading to information on the ways the atoms and molecules assemble on the nanoscale into larger structures. Indeed, nanotechnology is a natural extension and developments of micro technology, artificial intelligence and gene technology. Note that the spacing of atoms in a matter is about 1/100 of a nanometer and a strand of DNA is 2 nanometers wide and that a sheet of newspaper is 100,000 nanometers thick. Note also that nanoscience and nanotechnology includes a blending of developments in nano chemistry, nano biology, including the aspects of physics that are already valid at the level of elementary particles (i.e. at nano levels).

The start of modern day nanoscience and nanotechnology could be traced to the lecture given by Richard Feyman, a physicist, at the American Physical Society meeting at Caltex on December 29, 1959 titled “There is always a room at the bottom”. A crucial impetus for the growth of this field was provided in 1981 by G. Binnig and H. Rohrer when they invented the scanning tunneling microscope. Later, other types of scanning microscopes were created also for the manipulation and control of atoms and molecules. It is also noteworthy however, that M Knoll and E. Ruska had invented the electron microscope in 1931 and that in 1905 A. Einstein had estimated the diameter of sugar molecule as I nanometer.

Computational Nanoscience and Nanotechnology

Computational Nanoscience and Nanotechnology adopts mathematical and computer simulation techniques sometimes with experiments, to investigate existing nano materials as well as discover new ones. Computational techniques also help in studying, predicting and calculating properties and structure of molecules and other nanostructures. Although we shall discuss some of the techniques further in section 4, we now mention some of the computational methods used-e.g. Density Function Theory (DFT) developed by W. Kohn and J.A. Pople in 1965; Molecular Geometry and Molecular Mechanics; Molecular Dynamics, Molecular Quantum Mechanics including molecular Schrödinger equations and interpretations of the associated molecular wave functions: geometric optimization, Electron and charge distributions etc. As will be seen later , nanotechnology, which is classified mainly under high technologies in section 2, together with nanoscience encompass all the four areas of science and technology-Basic Sciences, Applied Sciences, Classical technology and High Technology--- which we view as concentric layers with diffuse boundaries with an inner core of basic sciences and mathematics as its innermost core. This invariably makes nanoscience and nanotechnology a highly multidisciplinary area of research, study and practice.

It is noteworthy that W. Kohn and J. A. Pople developed the Density function Theory (DFT) in 1965 and that J. Pople developed computational methods in quantum chemistry that same year. Fritz Heusler (1866-1947), Herman Weyl(1855-1955), and Michael Berry (1941-) are three renowned scientists whose work have provided important new insights into materials science, topology, and condensed matter physics , leading to the recent discovery of new and important quantum properties in new classes of nano materials which could lead new science. Heusler, in particular discovered compounds that are found to have non-trivial topological properties that could open a large field of new physics and mathematics. We shall discuss this further in sections 2 and 3.

Benefits of and Concerns Involved In Nanoscience and Nanotechnology

There are numerous benefits from Nano Science and nanotechnology –including health benefits, (treatment of a large variety of medical conditions—for example , new nano materials are designed and engineered that are suitable for medical implants and also silver nano particles with anti-microbial properties)); Economic benefits (over 110 billion dollars in sales by an industry manufacturing fine chemicals). However, there are several concerns connected with nanoscience and nanotechnology----nano particles can be inhaled and swallowed, and absorbed through the skin. Moreover, there are no adequate regulations regarding handling or labeling; there are health and environmental hazards; risks associated with molecular manufacturing; no law associated with intellectual property and there are also ethical issues.

Section Two

Mathematics Vis-À-Vis Other Areas of Science and Technology (Including Nanoscience and Nanotechnology)

Nature of mathematics

Some ramifications of mathematics

Several ramifications of mathematics include the following:

Number-which involves counting, measurements (e.g. of lengths, weights,) and the understanding of integers, real, complex numbers, and more sophisticated numbers like p-adic numbers etc.

Shape: e.g. triangles, circles, spheres, tetrahedron-leading to studies in geometries, topology, Lie groups and applications etc.

Movements: e.g. of planets and waves

Chance and Randomness-with its associated mathematics like probability, statistics, stochastic differential equations, etc.

Exploratory Powers Of New Technologies: e.g. computers, artificial intelligence, etc

Contemporary Mathematical Methods Rather Profound, Sophisticated, Technical and Diversified

Hence we have global illiteracy in contemporary mathematics resulting in hostilities from parents, government institutions, general public and some private sectors. All these raise serious pedagogical issues about teaching and learning of contemporary aspects of mathematics---hence a crying need for renovation of mathematics curricula at all levels. Many areas of basic sciences, applied sciences and technology--including Nanoscience and nanotechnology—now require sophisticated mathematics for their in-depth study.

The word "mathematical" which is sometimes used interchangeably with "theoretical" or "computational" is also inter-woven, by name, with other sciences. Thus we have e.g. Mathematical, (theoretical, computational) chemistry, physics, biology, economics, linguistics, material science, materials technology, nanoscience and nanotechnology etc.

The Four Components of Science and Technology

There are essentially four components of Science and Technology;--basic sciences, applied Sciences, Low or classical Technologies and Higher Technologies.

Basic Sciences

The basic sciences are: Mathematics (including statistics, and computer science), Physics, Chemistry and Biology (including basic medical sciences)

Applied Sciences

These include—Medicine and Health, Agriculture (including livestock, fisheries, and forestry studies), Earth Sciences (including meteorology, oceanography, irrigation and soils), Mineral exploration etc.

Low or Classical Technologies

These include: Iron steel and other metal goods, petroleum technologies, Power generation and transmission, Design and fabrication Industries.

High Technologies

These include: Micro-electronics(including software development, fabrication of microchips with industrial application), computer-aided design etc; space Sciences; New materials(including composite materials, and high temperature super conductors); Pharmaceuticals and fine chemicals; Biotechnology(including molecular biology, genetics and microbiology useful in agriculture, energy, medined); Nanotechnology in general etc.

Further Comments on Computational Nanoscience and Nanotechnology

Needless to say that global knowledge of Nanoscience and Nanotechnology has developed rapidly –thanks to the age of globalization that has made the world a global village. Indeed the contributions from nanoscience and nanotechnology to the world economy from industries for various fine chemicals alone amounted to over 110 billion dollars in sales in 2014. Health benefits have been tremendous. In terms of scientific benefits, the compounds discovered by Fritz Heusler long ago was recently found to host non-trivial topological (mathematical) properties that open a large field of new physics. Moreover, new and exciting quantum properties in new classes of nano-materials were recently discovered and could further lead to new science involving computing techniques and catalysis.

It is also clear from nature of mathematics to high technologies above that nanoscience and nanotechnology are highly multidisciplinary-being at the interface of many areas of basic sciences, applied sciences, classical and high technologies and so we could view nanoscience and nanotechnology (and indeed Science and Technology as in nature of mathematics to high technologies) as concentric layers with diffuse boundaries with a central core of basic sciences and mathematics at its innermost core-such that theories from the inner core help to solve problems in applied sciences as well as technology while problems arising from the outer layers of technology and applied sciences provide the inner cores of basic sciences and mathematics with new structures, new concepts and new methods.

The Role of ICT (Information Communications Technology)

The ICT components of various areas of science and Technology (including nanoscience and nanotechnology) have become more pronounced and prominent in this age of globalization. Indeed most recent developments all over the world have been ICT driven. Moreover, ICT has been used effectively to gather manipulate, present and communicate information all over the world.

More specifically: ICT has been bridging the technological divide between developed and the developing countries. The internet has facilitated easy flow of information. Smart phones of varying sophistication, Satellite TV networks, Electronic banking, Electronic Libraries, books and journals have now become a regular feature of life all over the world. Artificial intelligence and robotic technology are playing important roles in our industries as well as research and education outfits.

ICT-inspired village and cities are gradually springing up all over the world. Unifying themes in science and technology and in various disciplines must affect curriculum at all levels-education, health, agriculture, sconoics, etc. In fact, most global challenges can be translated into challenges involving S&T and ICT and hence mathematical sciences.

Section 3

Some Impacts of Mathematical Sciences on Other Areas of Science and Technology (Including Nanoscience and Nanotechnology)

In this section, we enumerate some of the sciences and technologies (including nanoscience and nanotechnology) that would not exist without mathematics.

Electrical Generation Technology

This is inspired by Faraday's theory of electricity and magnetism.

Wave Propagation, X-Rays, Radio, Television, Oil Exploration

These were inspired by Maxwell equations and Fourier analysis. Indeed Maxwell equations have led to the discovery of modern communication systems-radio, television etc whiles many electrical and electronic devices such as nuclear magnetic resonances and X-ray crystallographic spectrometers are based on Fourier analysis. Computational nanotechnology is based in parts on molecular Schrödinger equation together with its associated molecular wave propagation.

Acoustics, Electric Currents in the Brain, Turbulence, Stellar Structures

There are inspired by Fourier analysis and wavelet analysis.

Computer Revolution Is Mathematics Revolution

Computers are a creation of mathematics-Alan Turing's cogent and complete analysis of the notion of computation and logical proof of the existence of the universal computer. Computers are also creators of new areas of mathematics such as complexity theory, proof theory and Theory of algorithms. Moreover, computers have recorded tremendous success in the solution of outstanding mathematical problems e.g. four color problem, and classification of simple groups. Computers are useful for teaching mathematics,--calculus, matrix algebra, probability, statistics, geometry etc. They are also useful for solving problems arising in technology, commerce, business, economics etc. Moreover computerization of essential services--payment of salaries, banking, and library services, etc. has made life easier for all and sundry. Investigations in the direction of nanoscience and nanotechnology make use of mathematical and computer simulation skills to get results. For instance, computers are used to give information on properties of molecules or simulate experimental results or make predictions before actual experiments.

Subatomic Particles, Crystallography, Photochemistry, Etc.

These are inspired by Group Theory. We note also that subatomic particles have been greatly inspired by quantum mechanics and computer simulation.

Tracing of Hurricanes, Studying Aircraft Flight, Shocks in Non-Linear Waves

These can be modeled by Partial Differential Equations which can also be used to study vortices in fluid flows, blood flow through the heart, mixing of fuel in internal combustion engines, icebergs melting in the sea, crystal growth, and even the way in which radio telescope sense distant galaxies..

Communications, Urban Planning, Neurophysiology

These can be studied via graph theory, the mathematical study of networks.

Computational models of the heart, kidney, pancreas, and ear.

These can be modeled via Partial Differential Equations (PDE) and physiological fluid dynamics which is also useful is studying blood clotting, wave propagation of the inner ear, blood flow in the heart, cardiac chambers, arteries and veins, as well as air flow in lungs.

Green House Effect

This is the warming of the surfaces of the earth due to radiated energy of the "Greenhouse gases" such as methane from the atmosphere to the surface. The Greenhouse theory states that recent modification of the atmospheric gaseous composition will result in the gradual warming of the earth's surface as well as cooling of the upper atmosphere leading to a modification of the earth's climate. Numerical solutions of PDE are used to compute differences between a climate forced by increases in Greenhouse gases and a controlled climate.

Trajectory of Celestial Bodies, Meteorology

Modeling of this phenomena uses Ordinary Differential Equations,(ODE), Partial differential Equations (PDE), and Hamiltonian Mechanics.

Population Biology and Genetic Engineering

Population Biology has to do with counting, estimating, and predicting population sizes The problems involved range from managing of exhaustible resources like timber or fish, or even to geographical distribution of genes, age distribution of population ,genetic engineering and spread of forest and other resources. Mathematical theories involved include probability, dynamical systems, and wave propagation.

Investigation of Crimes

Mathematical techniques such as statistics, probability, wavelet analysis, image processing, and solving inverse problems (linking cause and effect) are central to modern forensic methods of investigation of crimes and bringing criminals to justice.

Section 4

More on Computational Nanoscience and Nanotechnology

In this small section, we briefly discuss some of the prominent mathematical methods used in computational Nanoscience and nanotechnology.

Quantum Physics and Molecular Schrodinger Equation

This method solves molecular Schrödinger equation associated with the molecular Hamiltonian.

Density Function Theory (DFT)

This method developed by W. Kohn and in 1965, is used for determining the molecular electronic structure.

Molecular Mechanics

This uses classical mechanics to model molecular structures. It can be used to study molecular systems ranging in size and complexity ranging from small to large biological systems or materials assembly with many thousands or millions of atoms.

Molecular Geometry

Molecular geometry is the three-dimensional arrangement of the atoms that constitute a molecule. It includes the general shape of the molecules, as well as bond lengths, bond angles and any other parameters that determine the position of each atom. The most popular methods for propagating the wave packet (envelope of localized wave action that travels as a unit) associated to the molecular geometry are1) split operator technique, 2) a sequence of polynomials which can be defined recursively,

Molecular Dynamics

This is used to calculate forces which are then used to solve Newton's law of motion to examine the time-dependent behavior of the nano particles.

Section 5

So far, Nano-Sceince and Nano-Technology (N&N) has made global tremendous progress within a relatively short time but there is a lot yet to be achieved and many concerns yet to be addressed. Here are some of them

1. New Generation of Catalysts Must Be Discovered

The use of solar and wind energy must be intensified to meet the world's demand for clean energy in the near future. There must be cheaper and better catalysts that can ensure the storage of solar and wind energy

2. Nano-materials at extreme conditions.

Develop enhanced capability of controlling nano materials at extreme conditions

3. Improve on Predictive Capabilities

In so doing, one would be enabling new technologies

4. Overcome Various Concerns, Challenges and Issues

These include health and environmental risk; social and ethical issues; regulation issues; risk associated with molecular manufacturing; intellectual property issues, etc.

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