

Computational Nanotechnology

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ABSTRACT

Nanotechnology has led to significant innovations in the diverse areas of electronics, microcomputing, and biotechnology to medicine, consumer supplies, aerospace, and energy production. Computational nanotechnology is the study, design, and optimization of nano-scale systems. It is a powerful tool for understanding nanoparticle physics and chemistry. It enables tools and techniques for physics-and-chemistry-based simulation. This paper provides a primer on computational nanotechnology.

INTRODUCTION

Nanotechnology, the science of tiny things at the nanoscale, may be the new frontier in the transformation of every sector, from medicine to the food industry. The 21st century is regarded as the century of nanotechnology. The applications of nanotechnology have become vast covering a wide range of fields including materials, electronics, photonics, biotechnology, life sciences, industry, food, agriculture, medicine, energy, transportation, defense/military, etc. The past two decades has witnessed how nanotechnology has progressed from academics and the laboratory research phase to use in various commercial applications. The research activities on nanotechnology are increasing globally at a rapid rate with almost no nation left behind. Industries and governments across the world are investing heavily in nanotechnology [1].

The development of algorithms and computational tools to the progress of nanoscience and nanotechnology have created an emerging research area known as computational nanotechnology. Computational nanotechnology (or computational nanoscience) arose in the 1990s as a synthesis of computational chemistry and computational nanotechnology, infused by people and practices from computational materials science, engineering, computer science, etc. Since then, computational nanotechnology has been a part of research. The goal of computational nanotechnology is to develop theory, models, and simulations [2].

In nanotechnology, computer simulations are important due to two main reasons. One is the difficulty in conducting actual experiments at this length scale. The second reason is that, even though in some cases the conventional theoretical models are valid, the inability to solve these models by incorporating all the complexities has brought in new challenges [3].

OVERVIEW OF NANOTECHNOLOGY

Nano is a prefix that indicates one billionth of a specified parameter. Nanotechnology is the engineering of systems at the molecular or nano scale. It has been called the second Industrial Revolution because of the special properties of materials at the nanoscale. It is a branch of green technology which has the potential to revolutionize many aspects of our lives. It has permeated all sectors of our economy due to the unique properties of materials at the nanoscale. It is transforming the world of materials and its influence will be broad. It will not only initiate the next industrial revolution, it will offer technological solutions. Nanocomputing is part of the emerging field of nanotechnology.

Richard Feynman, a famous Nobel Laureate physicist, is regarded as the father of nanotechnology. Nanotechnology has provided effective processing features, miniaturization from micro to nano obeying the Moore's law, which states that CPU is doubled in performance every 18 months [4]. Nanotechnology is the science of small things—at the atomic level or nanoscale level. It has the idea that the technology of the future will be built on atoms. It has impact on every area of science and technology [5].

Nanotechnology involves imaging, measuring, modeling, and manipulating matter at the nano scale. It covers a wide variety of disciplines like physics, chemistry, biology, biotechnology, information technology, engineering, and their potential applications.

Nanotechnology has a vast range of applications, such as in nanomedicine, nanoelectronics, biomaterials energy production, and consumer products. It is revolutionizing many industry sectors: information technology, homeland security, medicine, transportation, energy, food safety, and environmental science. In medicine, for example, nanotechnology is broadening the medical tools, knowledge, and therapies currently available to medical professionals. It can lead to creating smart drugs. Gold nanoparticles are being investigated as potential treatments for cancer and other diseases.

Nanoparticles are used increasingly in catalysis to boost chemical reactions, especially in petroleum refining and automotive catalytic converters. Nanotechnology will likely revolutionize sensor capabilities. Nanosensors and nanoactuators have the potential for improving the capability of sensor networks. Applications of nanotechnology are illustrated in Figure 1.

COMPUTATIONAL NANOTECHNOLOGY

Nanotechnology is applied in many scientific and practical applications, including medicine, agriculture, electronic devices, computer science, and many other fields. Figure 2 shows the subfields of computational nanotechnology [6]. Computational nanotechnology is used in predicting the toxicity caused due to different nanomaterials. It plays a major role in developing next generation of multifunctional materials, molecular scale electronic, and computing devices, sensors, actuators, and machines. Other applications of computational models in nanotechnology include the following [7]:

- *Medicine:* Computational models are used in various areas of medicine such as management of psychic disorders, cardiovascular diseases, brain diseases, cancer, diabetes, personalized medicine, etc. Computational modeling of physiological processes is crucial to comprehending complicated physiological phenomena accurately. Multiple computational techniques are utilized in medical field to create, improve, or to accelerate new drug development, creating the foundation of computer-aided medicine discovery. Computational

modeling techniques also help us understand the causes of disease at a profound level. Recently, the US Food and Drug Administration (FDA) used computational techniques to design different medical devices, which might aid in identifying and correcting issues during the formulation stage before the formulation is released into the market.

- *Drug Delivery*: Nanoscience and nanotechnology are perceived as a great potential to provide benefits in several areas such as the development of new drugs. Mathematical models have been used to explain experimental findings in drug delivery and extrapolate these experimental findings to larger populations. Computational models are applied in the development of nanoparticle and other organic and inorganic nanocarriers useful in drug delivery. Computational modeling has also shown its importance in pharmacokinetic studies.
- *Imaging*: Experimental methods and medical imaging advancements have shown the importance and application of computational modeling in the imaging study.
- *Nano-Engineered Electronic Device*: This involves developing computation and simulation tools that can be employed for turning nanoscale science and engineering into applications through the discovery and development of nanoelectronic-based devices.
- *Computational Nanoelectronics*: It develops and applies numerical algorithms to investigate nanodevices ranging from next generation transistors to thermoelectric generators and optoelectronic devices. While theories based on classical physics have been very successful in helping experimentalists design microelectronic devices, new approaches based on quantum mechanics are required to accurately model today nanoscale transistors and solar cells and to predict their characteristics even before they are fabricated.
- *Computational Nanomechanics*: The role of computational nanomechanics has become critically important in the cycle of growth and development of nanotechnology, because the length and time scales of important nanoscale systems and phenomenon have shrunk to the level, where they can be directly addressed, with high-fidelity computer simulations.

NETWORK FOR COMPUTATIONAL NANOTECHNOLOGY

The Network for Computational (NCN) is a multi-university center sponsored by the National Science Foundation to develop models and simulation tools to predict behavior at the device, circuit, and system level for nanoelectronics, nanoelectromechanics, and nanobio systems. Founded in 2002, the Network for Computational Nanotechnology (NCN) has pursued its mission to advance nanoscience and nanotechnology. The Purdue University-led cyber platform, nanoHUB, assists researchers across the globe by developing a virtual society. nanoHUB.org is recognized as the world's largest nanotechnology user facility. It facilitates fast knowledge transfer across countries, disciplines, and communities. Annually, nearly 250,000 users in 172 countries participate in nanoHUB, an online meeting place for simulation, research, collaboration, teaching, learning and publishing [8,9]. nanoHub is shown in Figure 3 [10].

The goals of NCN are to [11]: (1) accelerate the transformation of nanoscience to nanotechnology through the integration of simulation with experimentation; (2) engage an ever-larger and more diverse cyber community sharing novel, high-quality nanoscale computation and simulation research and educational resources; (3) develop open-access, open-source software to stimulate data sharing; and (4) inspire and educate the next-generation workforce. The NCN consists of a stand-alone Cyber Platform, which provides computation, simulation, and education services to over 330,000 researchers, educators, students, and industry members of the nanoscience and engineering community annually worldwide

BENEFITS

In this era, nanoscience progresses in every aspect of science, and nanotechnologies make life easier. Every research discipline benefits from nanotechnology, including physics, chemistry, biology, material science, computer science, and engineering. Nanotechnology has several advantages, such as superior surface area and nano-sized molecular structure. Nanomaterials have a higher energy storage capacity than coarse-grained compounds. It has capability to store high energy, which makes them applicable in the healthcare system. Computation modeling of nanocompounds is a powerful tool to identify their fundamental characteristics. As a result of the potential integration of photons, atoms, and biological cells via nanotechnology, new prospects have opened up for companies [7].

CHALLENGES

Although computational-modelling techniques are increasingly popular, there are challenges to overcome before they may be used in clinical practice. The integration of heterogeneous data from many sources and classes is a challenge. Computational modeling is regarded as less cumulative than other forms of study. It involves multiple simplifications, which may fail to capture all crucial features, creating issues associated with the model's validity. Some contend that computational models do not really advance our understanding because they are too complex to understand why they behave the way they do [7]. Improved technology is required to achieve a more robust quantitative understanding of matter at the nanoscale. Functional nanotechnology, nanoelectronics, nanofabrication, manufacturing, quantum engineering, and producing nanomaterials such as graphene and carbon nanotubes are all key skills that need to be developed.

CONCLUSION

Nanotechnology is the aptitude to perceive, measure, operate, and build materials at the nanometer scale, the size of atoms and molecules. It deals with materials, devices, and their applications, in areas such as engineered materials, electronics, computers, sensors, actuators, and machines, at the nano length-scale. It plays a growingly important role in understanding mechanical properties at such a small scale. Nanotechnology has promised a great future for humanity

Computational nanotechnology is emerging as a fundamental engineering analysis tool for the novel designs of nanodevices. It encompasses not only research into these exciting new computer technologies but also how to build them. This new manufacturing technology will usher in new possibilities in computation: molecular electronics, quantum cellular automata, DNA computing, single electron switches, adiabatic computing, quantum computing, and more. More information about computational nanotechnology can be found in the books in [1,12-24] and the following related journals:

- *Nanotechnology*
- *Computational Nanotechnology*
- *The IEEE Open Journal of Nanotechnology*
- *Journal of Computational and Theoretical Nanoscience*

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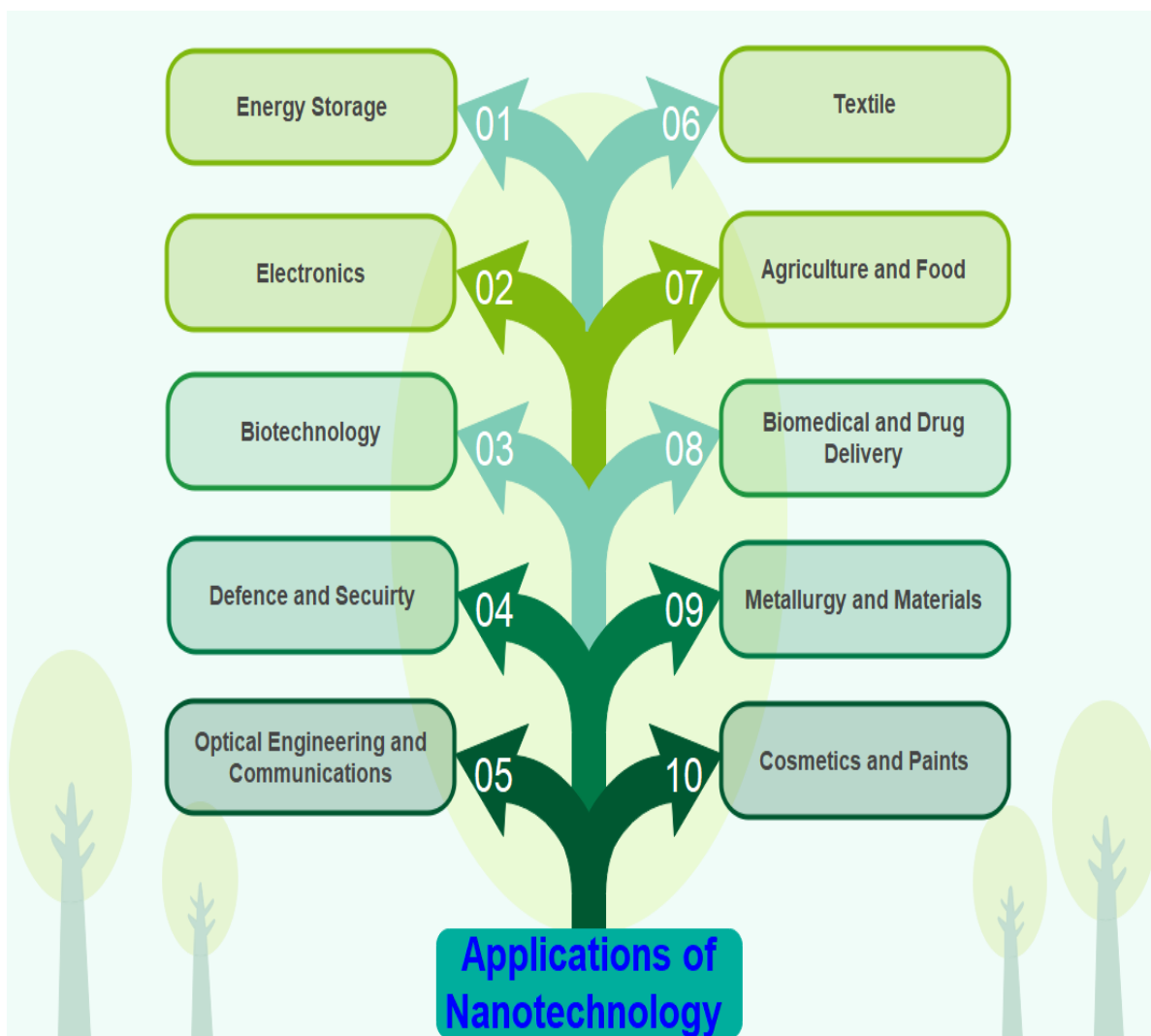


Figure 1 Applications of nanotechnology.

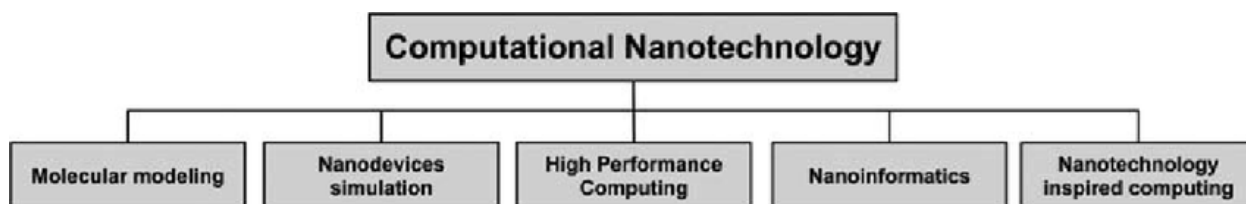


Figure 2 Subfields of computational nanotechnology [6].

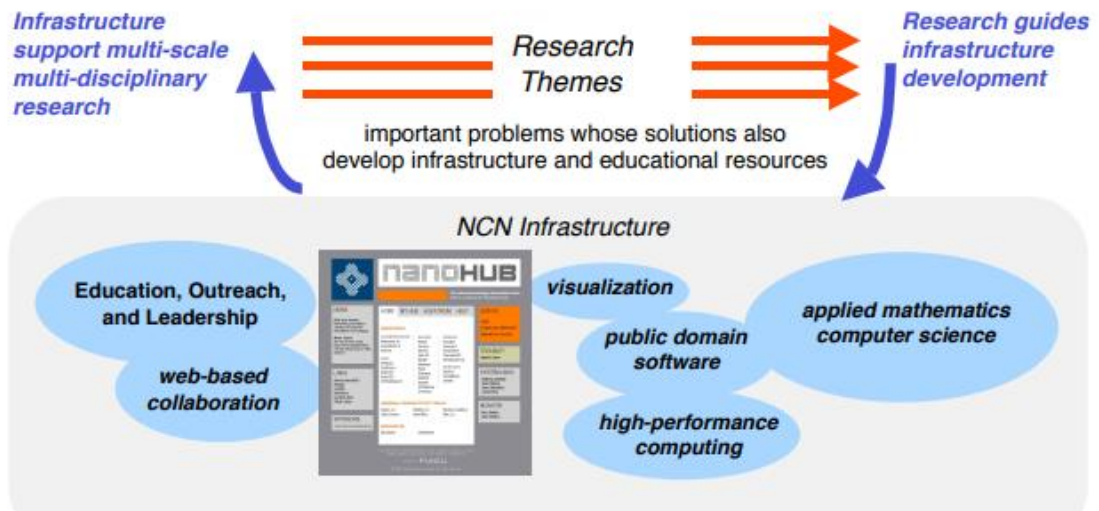


Figure 3 nanoHub [10].