

THE EMERGING ROLE OF NANOFINFORMATICS IN AMERICA

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ABSTRACT

The rapid expansion of nanotechnology coupled with its integration into different scientific domains has led to a new era. In recent decades, there has been an emergence of nanoinformatics in the USA and other European countries which deals with information science and nanotechnology. The present study reports the initiation and applicative properties of nanoinformatics in accordance to its scientific roles in America. In order to achieve the required milestone in nanoinformatics, there are major challenges that need to be addressed as scanty reports are available on nanoinformatics. Hence, the study highlights the importance of nanoinformatics in data curation and mining along with the role of governing bodies and the establishment of databases. These establishments are well organized to implement the untapped role of nanoinformatics which is rapidly growing. The information provided in the present mini- review adds scientific inputs towards the growing knowledge of nanotechnology and information science along with their future prospects.

KEYWORDS: Nanoinformatics, Information science, America, Nanotechnology.

INTRODUCTION

Over the last few years, the introduction of nanotechnological based applications has rapidly expanded (Baker et al., 2020). The technological aspect of nanotechnology has traded its application in all scientific domains (Syed et al., 2019). One of the least studied areas where scanty reports are available on the evaluation of nano aspects is information science (Afantitis et al., 2020). The combinatorial domains of both information science and nanotechnology offer significant advancement which can be termed as nanoinformatics (Liu and Cohen 2015). The field of nanoinformatics plays pivotal roles by integrating into different fields (Gonzalez-Nilo et al., 2011). For instance, designing computing platforms that can be used in predicting and screening of materials or chemical substances, developing national security sensors, development of web service with increased storage capacity and robust application, development of databases. etc. These technologies directly or indirectly become one of the major assets to any country across the globe.

America is one of the global leaders in technologies, implementation of nanoinformatics can boost different sectors. In recent years, there has been a collaboration of European commission along with the government of the United States to develop unique nanoinformatic material that can sense and interact with the biological system (Maojo et al., 2012). This project can provide, a great relief in designing drug discovery and act efficiently to enhance the existing medical applications. Further, in similar lines, there has been the development of a nanoinformatic tool that extracts, the information from the research articles and proposals using mining techniques which can add on more benefits to the biological databases and can overcome the laborious and time-consuming process (De la Iglesia et al., 2013, Pannerselvam and Choi, 2014). Also, America has always been upfront in the development of modern tools in the biomedical sector, usage of nanoinformatic principles can aid in designing onsite detection of disease kits, forecasting the early disease which aids in preventive measures, developing biosensors, etc (Sharma et al., 2015). Based on these brief facts and considerations, the present mini-review is designed to provide insight on nanoinformatics concerning its application in America.

NANOINFORMATICS IN DATA GENERATION

In America, the big data science has upgraded the new informative knowledge which has generated impute interest in myriad fields of science (Murtagh and Devlin, 2018). The introduction of nanotechnology has added value to these fields coupled with information science making it broader platforms. The nanoinformatic science has grabbed scientific attention in recent times owing to its accelerating scientific discovery to enable the facile route to overcome the risk assessment (Barnard et al., 2019). Some parameters are critical before the commercialization of products, for instance, leveraging research tools, initiating multiple tasks, translation of information, etc. To cope with these parameters, the integration of novel nano principles coupled with information science is implemented to come up with big data science with advanced technologies (Afantitis et al., 2020). For instance, in biomedical applications, the designing and illustration of nanomaterials to interact with the systems and provides insight on its mechanism and behavior can lead to designing novel strategies to improve the existing application, especially in drug designing. To screen, develop, and design a novel drug is bound with laborious work and time consuming which can lead to years. The use of novel informative science and nano-sized materials has uplifted the strategic value in designing and targeting specific sites that provide significant information and add value to big data science in the field of biomedical (Hulsen et al., 2019; Dash et al., 2019). Based on these principles and lines of interest, the National Cancer Institute collaborated with the nanotechnology working group to come up with the project National Cancer Informatics Program (NCIP) in 2008. The project is executed under the guidance of the CDC and FDA to translate information science with nanotechnology to upgrade the nanomedicine (Kuhnel et al., 2014). The project demonstrates in developing nanotechnology database which provides semantic search and provides information on the nanotoxicity. The pilot project is the hub of participants with researchers, academicians, governing bodies, and industries. Apart from this, there has been significant research being conducted to promote the information science with nanoparticles. According to the study conducted by Hendren et al., critical aspects of data generation were studied with the properties of nanoparticles, and their behavior was investigated. At the same time, the nano-safety and toxicity were also determined by the scientific community to come up with facile ways (Power et al., 2015). The nanoparticles were tuned in accordance with the data generation usage to maintain the quality and competitive standards were studied (Robinson et al 2016). The data generation and curation were generated to differentiate the parameters responsible for attenuating the properties of nanomaterials by studying the properties of nanomaterials (Oh et al, 2016). The already published data of nanomaterials was utilized to study the toxicity behavior and the role of functionalization and mode of synthetic data generation provided new insights to design and manipulate for the betterment of the society which led to increasing the applicative properties of the nanoparticles (Gernand and Casman, 2014).

NANOINFORMATICS IN DESIGNING AND MODELING

The use of information science in the biological system has demonstrated significant advances in studying the role of a specific structure or organs (Wooley and Lin, 2005). The study is based on the developing model and stimulation which provide information and its functional activities. These activities are recorded and data generation is executed. In recent years, the interaction of the nanoparticles with these biological systems is studied using an online modeling tool that comes in handy to predict the diseases cause and its management (Soares et al., 2018). There are myriad databases which cover a wide variety of study using automated and semi- automated modules (Azevedo et al., 2014). The nanoinformatics work in a sequence wherein the nanoparticles interact with the systems provides the knowledgeable outputs in the form of the proteomics, transcriptomics, and toxicological data which is curate using the modeling and automated tools which depict the signaling pathways and convert it into semantic schemes of data (Garcia-Remesal et al.,

2013; Karcher et al., 2018).

In America, the CDC and FDA are working together to implement and monitor projects working on nanoinformatics modeling which plays an immensely important role in developing novel drug targets for diseases like diabetes, antimicrobial resistance, cancer, and tuberculosis (Maojo et al., 2012; Pieters, and McKinney, 2013). This automated modeling helps in screening a large number of drug targets which predicts the beneficial aspect and toxicological behavior of the drug molecules. These results are deposited in the databases which envision the role of already tested molecules (Maojo et al., 2012). Apart from the screening protocol, the interaction of drugs with the specific organ in the body can be illustrated with these automated models and stimulation units which provide a clear picture on the pathway of the drug administered. In America, databases like NanosolveIT and eNanomapper are designed using the information gathered using the nanoinformatics tools (Maojo et al., 2012; Jeliazkova et al., 2015; Afantitis et al., 2020).

NANOINFORMATICS IN NATIONAL SECURITY AND SAFETY

In USA, the National Nanotechnology Initiative (NNI) was established in 2001 which has been working coordinating the research and development of nanotechnology-related projects (Sargent, 2014). The NNI constitutes 20 departments which enhances the research-related activities to support the goals by outlining the specific goal and fostering its activity (Plan 2007). In the NNI strategic plan, importance has been devoted to coordinate the national safety and security using nanotechnology coupled with existing scientific domains such as information science (Sargent, 2014). The NNI constitute a committee that shares the information related to national security and highlights the challenges faced. The nanoinformatics can act efficiently to protect the national interest of America, by designing tools and technology which can predict and diagnose the illegal activities with the help of a face recognition tool which provides the complete detailed information of the individual recorded in the databases (Plan 2007). These techniques are helpful in the borders, airports, and sensitive areas which can illustrate the threat for the nation in no time. Also, the nanoinformatics principles can be implemented to control the biological threat which often goes unrecognized. By providing the information of biowarfare agents enlisted in the databases. These tools can be handy for onsite detection and protection of national interest. The role of nanoinformatics plays an important role in advancing America's safety and security implementing the foreign policies which ensure the monitoring of foreign goods, people into the US territory (Plan 2007).

NANOINFORMATICS IN BIOMEDICAL APPLICATIONS

The use of information science tools can be traced down since the mid 19th century, wherein computers were used diagnostic techniques, information science-based radiology techniques, scanning tools were advanced with research and development (Liu and Cohen, 2015). The technology advanced with the more precise operation and detection tools for instance use of PCR and sequencer were able to generate accurate information at the molecular level providing more clear and authenticated information (Moajo et al., 2012). The introduction of nanotechnology in biomedical applications gained importance which was well received with the tools of information science. The technology improved with the collaborative approaches of two domains which resulted in the completion of the Human Genome Project giving the new horizon to developing more advanced software. In recent times, there has been tremendous interest in using nanoinformatics in biomedical applications with a large number of scientific groups working on this discipline. The techniques like targeted drug delivery systems were designed coupled with controlled release of drugs using nanoparticles. The effect was monitored and received using information science (Moajo et al., 2012). The result was studied and investigated to improve therapeutic efficacy, biocompatibility, and controlled released activity. Further, the use of nanoinformatics can be cited in early

diagnosing of life-threatening diseases such as cancer, organ failures, cardiovascular diseases, diabetics, etc (Moajo et al., 2012). In America, the diverse population with different races working along with the native every individual has different genetic makeup hence to improve the healthcare sector, CDC and FDA are coordinating the projects by providing the funding to improve the existing standards of the tools which are well received and implemented using the techniques of nanoinformatics (Moajo et al., 2012; Baciú et al., 2017).

NANOINFORMATICS IN DEVELOPMENT OF DATABASES

The development of databases is to provide accessibility of information available for the users for instance GenBank which provides the information of DNA sequences and protein structure database can be found in Protein Data Bank (Panneerselvam and Choi, 2014). Simultaneously, a large number of depositories and databases established such as NCBI and JSPS (Siva, 2009). All these databases led to a new era of information science bridging with other scientific domains. The emergence of bioinformatics displayed the importance of information tools (Dua and Chowriappa, 2012). The database for nanoinformatics is also established in a similar line, for instance, ISA-TAB -Nano, Nano-EHS database analysis tool, OECD, eNanomapper, caNanolab (Panneerselvam and Choi, 2014). Each database provides accessible information on the nanomaterials, their safety measures, and applicative properties.

NANOINFORMATICS IN ENVIRONMENTAL AND HEALTH PROCESSING

Every research should undergo the risk assessment of the environment and health care sectors. Nevertheless, nanoinformatics should be implemented with safe design to meet the applicative properties (Liu and Cohen, 2015). Hence, a large number of scientific data is collected to generate the physicochemical properties and effects of the nanomaterials which are processed and documented for curation and management (Comandella et al., 2020). The data is validated and analyzed to generate a nano database which is important for literature mining and big data analysis. The nanoinformatics assess the potential risk for environment and health with regards to the usage of nanoparticles in the process of application (Liu and Cohen, 2015).

NANOINFORMATICS IN DATA WAREHOUSE AND DATA MINING

To integrate the information of nanomaterials, data warehouse plays an important role. Currently, myriad tools and databases are already represented which are enabling the usage of data leading to a framework for big data science (Karcher et al., 2018). In nanotechnology, there have been challenges in designing the nanomaterials and to attenuate the applicative properties (Baker and Perianova, 2019). These challenges are met and processed with validation to foster the application and the data obtained and achieved are integrated within the particular discipline. The data warehouse and mining provide data implementation, workflow, curation, and analysis (Karcher et al., 2018). Hence to monitor the data integration, NDCI is currently coordinating and expanding the road map. The nanoinformatics is a broad domain which can yield unusual results which are executed into deeper data mining process (Hendren et al., 2015).

NANOINFORMATICS IN MANUFACTURING OF DEVICES

The use of nanoinformatics principles in manufacturing devices has long driven with innovating applicative properties (Afantitis et al., 2020). For instance, the development of a sensing device is integrated with nanomaterials to detect the analyte at the trace level (Baker et al., 2012). This principle can be used to monitor illegal smuggling goods, environmental contaminants, rapid detection tools for a specific disease in the biomedical field (Baker et al.2012). The construction of these sensors is integrated with information

science tools that provide a rapid sensing process. Also, there has been the usage of nanomaterials coupled with sensing devices in developing chip-based trackers which can help in monitoring the movement of the desired object. Hence, nanoinformatics plays an important role in manufacturing nanodevices for modern applications (Baker et al., 2012; Afantitis et al., 2020).

FUTURE PROSPECTIVE OF NANOINFORMATICS

The nanoinformatics is an emerging field of science, which is growing at a rapid pace and trading its applications in different sectors. In order to achieve the required milestone, there are major challenges which need to be addressed such as scanty data availability on nanoinformatics as it is an emerging field of science, required user-friendly construction of computational software and models, need to validate and test the nanomaterials and its toxicity prior to the implementation of nanoinformatics and its usage at the wider range is a crucial factor. Recently, the US and other European countries have emerged with a roadmap 2030 to expand the application of nanoinformatics in order to monitor and study the risk assessment and governance. This road map can account to find the research gap and fill accordingly to foster the impact of nanoinformatics in modern society. However, a large number of scientific studies need to be implemented in order to reach the benefit of nanoinformatics in remote areas and developing countries. Hence, the USA is leading from the front to promote the concept of nanoinformatics for the betterment of society. The present review was drafted and executed to highlight the importance of nanoinformatics in the different sectors with respect to the role of America in disseminating the concept and knowledge.

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