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Nanoinformatics: A Conjecture and a Review.

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ABSTRACT

Nanoscience and technology is now widened its surface area in its solid ground and it is regarded as very spectacular amount among science scholars and even laymen. Nanoinformatics is an application which encompasses nanoscience and information & communication technology. Nano materials produced as of now should be documented properly, for that we need an effective communication tool, in this review we have presented a speculative idea to use ICT to document the nanoscience related issues and can predict the product as before the synthesis. Nanoinformatics has recently come out to address the need of computing applications of nanomaterials. While nanomaterials open up the possibility for developing new advantages in many industrial and scientific areas, they also offer leap forwarding perspectives for the prevention, diagnosis and treatment of diseases. In this review, we analyze the different aspects of nanoinformatics and catalyze new research and development. We also take-in the use of informatics to further the biological and clinical applications of basic research in nanoscience and nanotechnology, and the related concept of an extended "nanotype" to combine information related to nanoparticles.

Keywords: Nanoscience and technology, information & communication technology, Nanoinformatics, computing applications and nanoparticles.

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INTRODUCTION

Over the last decades Nanotechnology has promised to advance science and technology in many areas. Within medicine, Nanomedicine promises to deliver new methods for diagnosis, prognosis and therapy. As the amount of available information is rapidly growing, new Biomedical Informatics approaches have to be developed to satisfy the increasing demand on data and knowledge management. In Europe, a project named ACTION-Grid was launched in 2008 with support from the European Commission to analyze the challenges and agenda for developing Nanoinformatics as a discipline related to Nanotechnology, Biomedicine and Informatics. Nanoinformatics aims to create a bridge between Nanomedicine and Information Technology applying computational methods to manage the information created in the nanomedical domain. Nanoinformatics could expand previous experiences in Biomedical Informatics with new features required to study different scientific biological and physical characteristics at a different level of complexity. ACTION-Grid is a project, funded by the European Commission, which aims to the creation of a collaborative environment in biomedical and nanomedical research among countries in Europe, Western Balkans, Latin America and North Africa. In this paper, we briefly review the concepts of nanomedicine and nanoinformatics and then we describe the activities of some of the ACTION-Grid consortium members considering those initiatives related to nanomedicine.

Information and communication technology (ICT)

ICT is often used as an extended synonym for information technology (IT), but is a more specific term that stresses the role of unified communications and the integration of telecommunications (telephone lines and wireless signals), computers as well as necessary enterprise software, middleware, storage, and audio-visual systems, which enable users to access, store, transmit, and manipulate information.The term *ICT* is also used to refer to the convergence of audio-visual and telephone networks with computer networks through a single cabling or link system. There are large economic incentives (huge cost savings due to elimination of the telephone network) to merge the telephone network with the computer network system using a single unified system of cabling, signal distribution and management.

The phrase Information and Communication Technology has been used by academic researchers in the 1980s [3]. The term ICT became popular after it was used in a report to the UK government in 1997 and in the revised National Curriculum for England, Wales and Northern Ireland in 2000[4]. But in 2012, the Royal Society recommended that the term ICT should no longer be used in British schools "as it has attracted too many negative connotations"[5]. Then with effect from 2014 the National Curriculum was changed to use the word computing which reflects the addition of computer programming to the curriculum [6].

The term is commonly used as a synonym for computers and computer networks, but it also encompasses other information distribution technologies such as television and telephones. Several industries are associated with information technology, including computer hardware, software, electronics, semiconductors, internet, telecom equipment, e-commerce and computer services[7]. Humans have been storing, retrieving, manipulating and communicating information since the Sumerians in Mesopotamia developed writing in about 3000 BC, but the term *information technology* in its modern sense first appeared in a 1958 article published in the *Harvard Business Review*; authors Harold J. Leavitt and Thomas L. Whisler commented that "the new technology does not yet have a single established name. We shall call it information technology (IT)." Their definition consists of three categories: techniques for processing, the application of statistical and mathematical methods to decision-making, and the simulation of higher-order thinking through computer programs [8].

Bioinformatics and cheminformatics

Bioinformatics is an interdisciplinary field that develops methods and software tools for understanding biological data. As an interdisciplinary field of science, bioinformatics combines computer science, statistics, mathematics, and engineering to study and process biological data [9]. Bioinformatics is both an umbrella term for the body of biological studies that use computer programming as part of their methodology, as well as a reference to specific analysis "pipelines" that are repeatedly used, particularly in the fields of genetics and genomics. Common uses of bioinformatics include the identification of candidate genes and nucleotides (SNPs). Often, such identification is made with the aim of better understanding the genetic

basis of disease, unique adaptations, desirable properties (esp. in agricultural species), or differences between populations. In a less formal way, bioinformatics also tries to understand the organisational principles within nucleic acid and protein sequences [10].

To study how normal cellular activities are altered in different disease states, the biological data must be combined to form a comprehensive picture of these activities. Therefore, the field of bioinformatics has evolved such that the most pressing task now involves the analysis and interpretation of various types of data. This includes nucleotide and amino acid sequences, protein domains, and protein structures. The actual process of analyzing and interpreting data is referred to as computational biology. Important sub-disciplines within bioinformatics and computational biology include:

1. Development and implementation of computer programs that enable efficient access to use and manage various types of information.

2. Development of new algorithms (mathematical formulas) and statistical measures that assess relationships among members of large data sets. For example, there are methods to locate a gene within a sequence, to predict protein structure and/or function, and to cluster protein sequences into families of related sequences.

The primary goal of bioinformatics is to increase the understanding of biological processes. What sets it apart from other approaches, however, is its focus on developing and applying computationally intensive techniques to achieve this goal. Examples include: pattern recognition, data mining, machine learning algorithms, and visualization [11]. Major research efforts in the field include sequence alignment, gene finding, genome assembly, drug design, drug discovery, protein structure alignment, protein structure prediction, prediction of gene expression and protein–protein interactions, genome-wide association studies, and the modeling of evolution. Bioinformatics now entails the creation and advancement of databases, algorithms, computational and statistical techniques, and theory to solve formal and practical problems arising from the management and analysis of biological data. Over the past few decades rapid developments in genomic and other molecular research technologies and developments in information technologies have combined to produce a tremendous amount of information related to molecular biology. Bioinformatics is the name given to these mathematical and computing approaches used to glean understanding of biological processes [12].

Cheminformatics combines the scientific working fields of chemistry, computer science and information science for example in the areas of topology, chemical graph theory, information retrieval and data mining in the chemical space. Cheminformatics can also be applied to data analysis for various industries like paper and pulp, dyes and such allied industries [13]. The primary application of cheminformatics is in the storage, indexing and search of information relating to compounds. The efficient search of such stored information includes topics that are dealt with in computer science as data mining, information retrieval, information extraction and machine learning. Related research topics include: Unstructured data, Information retrieval, Information extraction, Structured Data Mining and mining of Structured data, Database mining, Graph mining, Molecule mining, Sequence mining and Tree mining[14].

Nanoscience and technology

Nanotechnology ("nanotech") is the manipulation of matter on an atomic, molecular, and supramolecular scale. The earliest, widespread description of nanotechnology referred to the particular technological goal of precisely manipulating atoms and molecules for fabrication of macroscale products, also now referred to as molecular nanotechnology[1][2]. A more generalized description of nanotechnology was subsequently established by the National Nanotechnology Initiative, which defines nanotechnology as the manipulation of matter with at least one dimension sized from 1 to 100 nanometers. This definition reflects the fact that quantum mechanical effects are important at this quantum-realm scale, and so the definition shifted from a particular technological goal to a research category inclusive of all types of research and technologies that deal with the special properties of matter that occur below the given size threshold. It is therefore common to see the plural form "nanotechnologies" as well as "nanoscale technologies" to refer to the broad range of research and applications whose common trait is size. Because of the variety of potential applications (including industrial and military), governments have invested billions of dollars in

nanotechnology research. Through its National Nanotechnology Initiative, the USA has invested 3.7 billion dollars. The European Union has invested 1.2 billion and Japan 750 million dollars [3].

Nanotechnology as defined by size is naturally very broad, including fields of science as diverse as surface science,organic chemistry, molecular biology, semiconductor physics, microfabrication, etc [4]. The associated research and applications are equally diverse, ranging from extensions of conventional device physics to completely new approaches based upon molecular self-assembly, from developing new materials with dimensions on the nanoscale to direct control of matter on the atomic scale.

Scientists currently debate the future implications of nanotechnology. Nanotechnology may be able to create many new materials and devices with a vast range of applications, such as in medicine, electronics, biomaterials energy production, and consumer products. On the other hand, nanotechnology raises many of the same issues as any new technology, including concerns about the toxicity and environmental impact of nanomaterials, and their potential effects on global economics, as well as speculation about various doomsday scenarios [5]. These concerns have led to a debate among advocacy groups and governments on whether special regulation of nanotechnology is warranted.

Speculative

These subfields seek to anticipate what inventions nanotechnology might yield, or attempt to propose an agenda along which inquiry might progress. These often take a big-picture view of nanotechnology, with more emphasis on its societal implications than the details of how such inventions could actually be created [6].

- Molecular nanotechnology is a proposed approach which involves manipulating single molecules in finely controlled, deterministic ways. This is more theoretical than the other subfields, and many of its proposed techniques are beyond current capabilities.

- Nanorobotics centers on self-sufficient machines of some functionality operating at the nanoscale. There are hopes for applying nanorobots in medicine,but it may not be easy to do such a thing because of several drawbacks of such devices. Nevertheless, progress on innovative materials and methodologies has been demonstrated with some patents granted about new nanomanufacturing devices for future commercial applications, which also progressively helps in the development towards nanorobots with the use of embedded nanobioelectronics concepts [14].

- Productive nanosystems are "systems of nanosystems" which will be complex nanosystems that produce atomically precise parts for other nanosystems, not necessarily using novel nanoscale-emergent properties, but well-understood fundamentals of manufacturing. Because of the discrete (i.e. atomic) nature of matter and the possibility of exponential growth, this stage is seen as the basis of another industrial revolution. Mihail Roco, one of the architects of the USA's National Nanotechnology Initiative, has proposed four states of nanotechnology that seem to parallel the technical progress of the Industrial Revolution, progressing from passive nanostructures to active nanodevices to complex nanomachines and ultimately to productive nanosystems [15].

- Programmable matter seeks to design materials whose properties can be easily, reversibly and externally controlled though a fusion of information science andmaterials science.
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- Due to the popularity and media exposure of the term nanotechnology, the words picotechnology and femtotechnology have been coined in analogy to it, although these are only used rarely and informally.

Nanoinformatics

Nanoinformatics is the science and practice of determining which information is relevant to the nanoscale science and engineering community, and then developing and implementing effective mechanisms for collecting, validating, storing, sharing, analyzing, modeling, and applying that information. Nanoinformatics also involves the utilization of networked communication tools to launch and support efficient communities of

practice. Nanoinformatics is necessary for intelligent development and comparative characterization of nanomaterials, for design and use of optimized nanodevices and nanosystems, and for development of advanced instrumentation and manufacturing processes. Nanoinformatics also fosters efficient scientific discovery and learning through data mining and machine learning techniques. A Roadmap for Nanoinformatics [16].

The Nanoinformatics 2020 Roadmap [April 2011] is a community-owned program for developing coordinated activities in multiple subdomains of nanotechnology that are both complementary and lead to community-wide standards and tools for ongoing research and development of nanotechnology. This roadmap will be the first broad-based community effort to articulate comprehensive needs and goals for nanoinformatics. This effort responds to the call for roadmaps in the National Nanotechnology Initiative Strategic Plan.

The Nanoinformatics 2020 Roadmap is based in part on Nanoinformatics 2010, a collaborative roadmapping workshop and key component of this overarching roadmapping project. Nanoinformatics 2010 was planned around the belief that cooperation between disciplines and organizations and the advancement of nanotechnology research and development can be facilitated through informatics efforts. The program itself was designed to bring together diverse disciplinary-based approaches to the workshop themes; to showcase nanoinformatics tools and projects; to discuss challenges associated with each theme; and to enable the community to sketch out a path for addressing the grand challenges of nanotechnology through e-Science. Nanoinformatics 2010 and its outcomes are described as part of the Nanoinformatics 2020 Roadmap [17].

CONCLUSION

At the conclusion we suggest that nanoinformatics is an emerging science which could be extensively utilized to evolve with novel drugs and can be used to conserve nano information.

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