Nanoinformatics: new challenges for biomedical informatics at the nano level

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Nanoinformatics: New Challenges for Biomedical Informatics at the nano level

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Abstract. 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 2007, a new subdiscipline, already named "Nanoinformatics", has been created with support from the US National Science Foundation. In Europe, a project named ACTION Grid has been launched with support from the European Commission to analyze challenges and agenda for developing Nanoinformatics as a discipline related to Nanotechnology, Bio-medicine and Informatics. For MIE 2009, members of this consortium proposed a Workshop to discuss the scientific and strategic issues associated to this topic. Nanoinformatics aims to create a bridge between nanomedicine and information technology applying computational methods to manage the information created in the nanomedical domain.

Keywords. Nanoinformatics, Nanomedicine, Biomedical informatics.

Introduction

Nanotechnology aims to advance the formulation of materials and manufacture of devices by controlling matter at the scale of 1-100 nanometers. The novel properties of the resulted nano-materials and the induced phenomena could be exploited towards significant medical applications, such as for the diagnosis and therapy of diseases, in an already established discipline named Nanomedicine. A new discipline, Nanoinformatics, is currently being developed in parallel to address the informatics needs of Nanomedicine. From a Biomedical Informatics, it could be the continuation of Biomedical Informatics at the atom level, opening a significant range of applications and scientific research. In such direction, authors of this paper have proposed a Workshops to be carried out at the MIE 2009 conference, where all these issues could be discussed. This continues efforts already launched by the European Commission and the US National Science Foundation.

1. Nanomedicine

As nanomedicine begins to define itself, new interesting research directions are opened to the scientific community. Examples of the possibilities of nanomedicine are the achievement of non-damaging observation and diagnostic modalities or nano-devices and innovative tools for understanding cell mechanisms or differences between normal and abnormal physiological states. Nanodevices allow the analysis (on high sensitivity levels) of relatively small sample volumes enabling the acquisition and manipulation of cellular parameters (regarding cellular mechanics, morphology, and cytoskeleton), which have been hard to achieve using conventional technology [1].

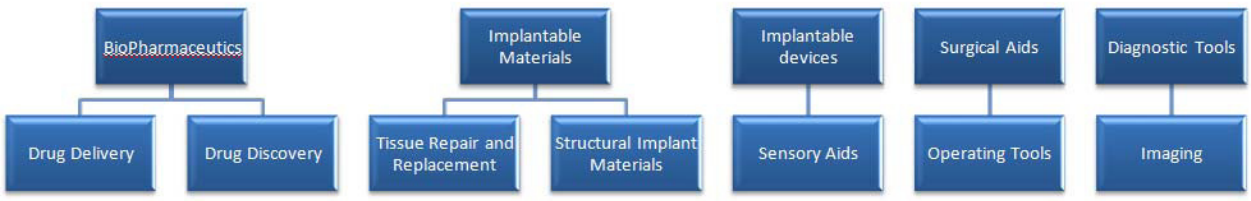

Fig 1. A representation of different aspects of Nanomedicine [2]

Nanomedicine can bring to such aspects of diagnosis, prognosis and treatment processes results that traditional medicine could not even foresee. Complex molecules that seek out diseased or cancerous cells, sensors for diagnosing diseased states or replacement therapy may open new horizons for medicine.

2. Nanoparticles in medicine

Nanoparticles and nanomaterials are built as biodetection agents for DNA and proteins. In addition, nanodevices, such as nanowires and nanotubes, can be combined with nanoarrays to create automated nanodetection platforms. The MeSH term "nanoparticle" was introduced in
2007, described as follows: "Nanometer-sized particles that are nanoscale in three dimensions. Term nanoparticle is
subordinated to term nanostructure and superordinated to several terms: Dendrimers, Metal Nanoparticles,
Nanocapsules, Nanosphere and Quantum Dots"[3].

Fig 2. "Nanostructures" in MeSH

All these kinds of nanoparticles can be used in nanomedicine for different purposes. Dendrimers and nanospheres can be used as drug carriers or Quantum Dots can be used as marker for diagnosis and monitoring tasks. In general we can anticipate that nanoparticles will have a primary role in medical research within the next decades. However, the scientific community also faces some questions about patient safety and other possible secondary effects, such as those related to the use of nanoparticles. Studies on possible risks for human health due to the use of nanoparticles are currently obtaining an increasing interest. Nanoparticles can be of natural or biological origin, —like viruses—, and engineered —i.e. of nonbiological origin. Viruses can be more or less invasive, and can cause serious health problems in human, animals or plants, in many cases more serious than bacterial organisms do. However, it can be argued that the non biological nanoparticles may produce similar or even greater damages. If this happened, how to handle them?

The new area of Nanotoxicology wants to answer questions like those mentioned above. Research in this direction will be fundamental to ensure safe uses of nanoparticle-based medical products. To carry out experiments, new models of clinical trials will be needed. For all these issues, medical information will have to be linked to these experiments. In this direction, Nanoinformatics may play a significant role.

3. Nanoinformatics

Nanoinformatics is a new discipline that has grown exponentially over the last year, showing an interest in the computational aspects related to Nanotecnology and, obviously, Nanomedicine. Nanoinformatics can be seen as the extension of Biomedical Informatics at the atomic scale —although there are singularities that need to be analyzed.

Nanoinformatics describes the application of computer technology, information science and molecular simulations to organize, interpret, and predict the structure and physico-chemical properties of nanoparticules and nanomaterials. While Bioinformatics is usually applied in the context of analyzing DNA sequence data, Nanoinformatics is applied in the context of characterizing particles and materials with application in nano and biotechnology. A nanoinformatics key issue is the linkage of

information, data, results and findings acquired using nano-related processes with the standard clinical procedures. This task will be fundamental for the future evolutions of the medical area.

Figure 3 shows below an example of such extended vision of Biomedical Informatics towards the Nano level, into this area of Nanoinformatics. During the last decade there have been many efforts to link the classical areas of Medical Informatics and Bioinformatics. This effort has been boosted by results from various genomic projects, producing 1000+ databases with "-omics" data that are currently used for research. The areas of genomic and personalized medicine and translational bioinformatics, which aims to transfer results of basic research to different new direction in medicine are good examples of such synergy. Meanwhile, the "Nano" level opens up new directions and challenges, for basic and applied research, that should be thoroughly discussed. The workshop at the MIE 2009 plans to directly analyse these questions and their particular relevance for the Biomedical Informatics Agenda.

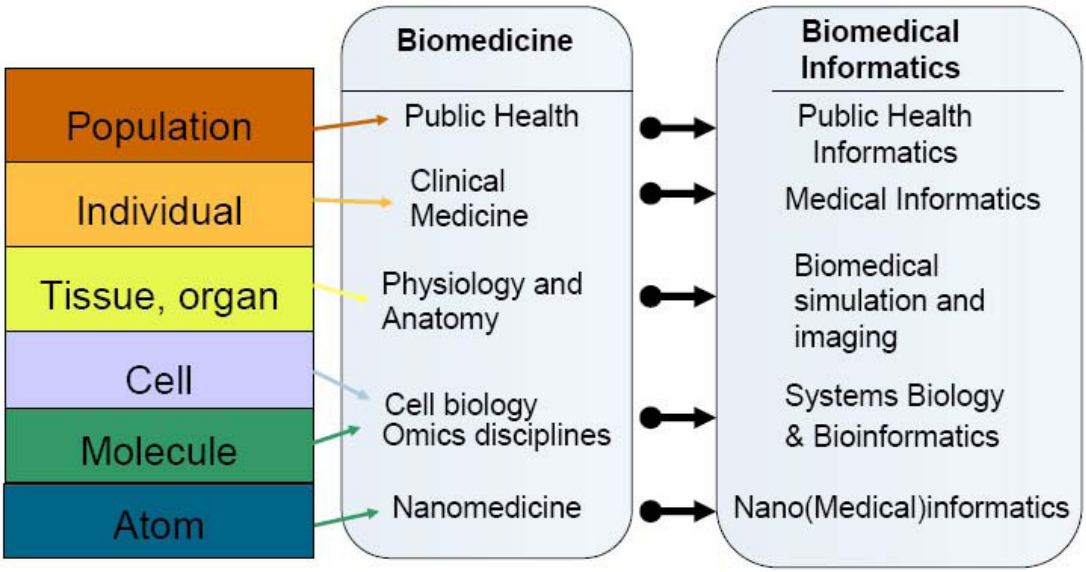

Figure 3. Biomedical informatics going down to the atom level, towards Nanoinformatics. (extracted from [4])

4. The ACTION-Grid project

ACTION-Grid [5] is a project that aims to establish the basis for a dialogue among researchers in Medical Informatics, Bioinformatics and Nanoinformatics. The project involves countries belonging to four different geographic areas: Europe, The Western Balkans, Latin America and North Africa.

One of ACTION-Grid's main goals is to provide information about the informational resources used and created by professional researchers in the disciplines mentioned before. By sharing this information, the scientific community can collaboratively develop better databases, tools or services (in general "resources) that others already created and that can be used by others researchers.

A second important objective of the project is to identify the most relevant research directions in Medical Informatics, Bioinformatics and Nanoinformatics. The results of this task will be used by the European Commission as a roadmap for future project Calls.

At the same time, partners of the ACTION-Grid project are currently working on different Nanoinformatics initiatives such as:

- Develop a method for the automatic creation and update of the resource index mentioned before [6]
- Research on Micro and Nano arrays
- Studies on Lab-on-Chip technologies [7]
- Adaptation of knowledge management systems to the nanomedicine context [8]
- A database of nanoparticles for national agencies

5. Conclusions

Nanoinformatics represents a new stage in the Biomedical Informatics area. While knowledge about nanotechnology is constantly increasing, the importance of the synergy between “nano” and “info” domains is just beginning. Thus, it is fundamental for the scientific community to work on the analysis and the development of the potentialities of this discipline. For Biomedical Informatics professionals, there will be a large number of issues to be discussed and addressed in the next decades. These issues could lead to open up complete new areas of research and development.

This proposal, summarizing in part previous documents and work carried out by ACTION-Grid members, aims to invite researchers to discuss these issues in an open workshop at the MIE 2009 conference. In this event researchers will discuss scientific and technological challenges in the area and proposals for future work at the European level. Similar initiatives have recently begun with support by important national and international organizations [9, 10, 11].

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