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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 sub-discipline, already named "Nanoinformatics", was created with support from the US National Science Foundation. 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. For MIE 2009, members of this consortium proposed a workshop to discuss the scientific and strategic issues associated with 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

1. 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 nanomaterials and the induced phenomena can be exploited for significant medical applications including; the scientific discipline related to these topics is called Nanomedicine. A new scientific discipline, Nanoinformatics, is currently being developed in parallel to address the informatics needs of Nanomedicine. Nanomedical Informatics can be considered the extension of Biomedical Informatics at the atomic level, opening a new and significant range for applications and informatics research.

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The authors of this paper have proposed a workshop to be carried out at the MIE 2009 conference where these issues will be discussed. This workshop continues efforts already launched by the European Commission and the US National Science Foundation. In the next sections we provide an overview about the scientific challenges that will be addressed in the workshop.

2. Nanomedicine

As Nanomedicine begins to be defined, new interesting research directions are opened to the scientific community. Examples of the possibilities of Nanomedicine are the achievement of nanodevices (non-damaging observation and diagnostic modalities) for understanding cell mechanisms or differences between normal and abnormal physiological states. Nanodevices allow a high sensitivity analysis of relatively small sample volumes thus enabling the acquisition and manipulation of cellular parameters (regarding cellular mechanics, morphology, and cytoskeleton). This is difficult to achieve using conventional technology [1].

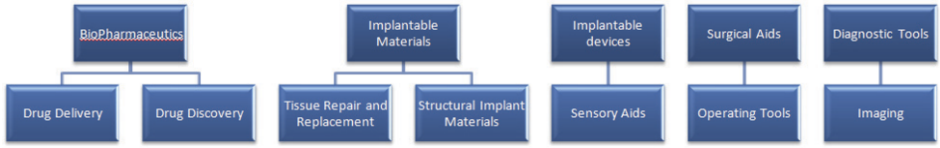

Figure 1. A representation of different aspects of Nanomedicine [2]

Nanomedicine can bring results to aspects of diagnosis, prognosis and treatment processes that traditional medicine could not even foresee. New horizons for medicine are being opened by Nanomedicine's focus on complex molecules that seek out diseased or cancerous cells, sensors for diagnosing diseased states, replacement therapy, and other topics (see Figure 1).

2.1. 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 and is 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, nanospheres and quantum dots" [3]. All of these kinds of nanoparticles can be used in Nanomedicine for different purposes. Dendrimers and nanospheres can be used as drug carriers. Quantum dots can be used as markers for diagnosis and monitoring tasks. We can anticipate that nanoparticles will have a primary role in medical research within the next decade and that Nanomedicine will become part of routine medical care.

However, the scientific community also faces some questions about patient safety and other possible secondary effects related to the use of nanoparticles. Studies on possible risks for human health due to the use of nanoparticles are gathering increasing interest. Nanoparticles can be of natural or biological origin – like viruses – and

engineered – i.e., of non-biological origins. Scientists argue that the non biological nanoparticles may produce similar or even greater damage compared to biological nanosize agents such as viruses [4]. This concern warrants prospective monitoring of nanomaterial experiments and research studies focused on such. The new area of Nanotoxicology focused on such issues. In this domain, Nanoinformatics may play a significant role, helping to process data extracted by tests and specifically designed clinical trials.

3. Nanoinformatics

Nanoinformatics is a new discipline that has grown exponentially over the last two years, showing an interest in the informatics and computational aspects related to Nanotechnology 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 nanoparticles and nanomaterials. While Bioinformatics is usually applied in the context of analyzing DNA sequence and other biomolecular 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. Ultimately this information will be part of treatment modalities and represented in electronic medical records. The discussion of the possibilities offered by this integration process is one of the scientific challenges addressed by the workshop.

Figure 2 shows an 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 applications 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.

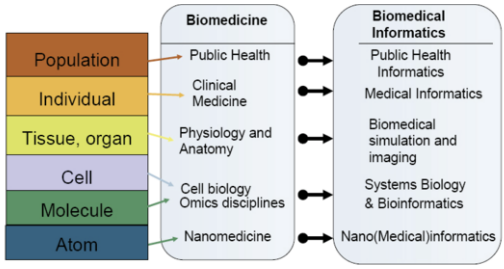

Figure 2. Biomedical informatics extended to the atom level, towards nanoinformatics (extracted from [5])

4. The ACTION-Grid Project

ACTION-Grid [6] 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 mentioned disciplines. By sharing this information, the scientific community can collaboratively develop better databases, tools or services 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 EC 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:

- Development of a method for the automatic creation and update of available resources [7]
- Research on Micro and Nano arrays
- Studies on Lab-on-Chip technologies [8]
- Adaptation of knowledge management systems to Nanomedicine [9]
- 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 the "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 completely 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 the workshop, 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 the support of important national and international organizations [10–12].

6. Workshop Organization

The workshop will introduce the concept of Nanomedical Informatics, offering an overview of the current efforts for defining this discipline. The workshop faculty will describe some of the current initiatives that involve Nanoinformatics in different geographical areas and different scientific contexts. It will offer presentations in which experts from different countries will introduce specific topics, followed by a discussion session and round tables in which participants will be able to interact with the experts.

The workshop does not strictly require any prerequisite. Basic knowledge of informatics, Nanotechnology, Nanomedicine and Bioinformatics may be useful for a deeper understand of the presentations. Addressed audience is all scientists interested in nano-bio-medical areas.

6.1. Expected Results

The workshop wants to gather the attention of the scientific community on Nanoinformatics. Providing a general vision of the discipline, its main challenges and future perspectives, the workshop will define the basis for a wider and deeper discussion about this topic. Finally this workshop is expected to discuss the most relevant issues in this area, including training needs and data organization issues.

6.2. Invited Speakers

At the date in which this document is written, the following researchers have agreed to participate in the workshop:

- Josipa Kern (Director of HMIG, University Zagreb Medical School, Croatia)
- Victor Maojo (Director of the Medical Bioinformatics Group at UPM, Spain)
- Fernando Martín-Sanchez (Vice-President of IMIA, Head of Medical Bioinformatics Department at ISCIII, Spain)
- George Potamias (Senior researcher at FORTH, Greece)
- Vassilis Moustakis (Senior researcher at FORTH, Greece)
- Joyce A. Mitchell (Chair of Biomedical Informatics Department, University of Utah, US)

Their presentations will be about topics mentioned above in this document.

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